

THE TIME-DEPENDENT HARTREE-FOCK-BOGOLIUBOV EQUATIONS FOR BOSONS

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ABSTRACT. In this article, we use quasifree reduction to derive the time-dependent Hartree-Fock-Bogoliubov (HFB) equations describing the dynamics of quantum fluctuations around a Bose-Einstein condensate in \mathbb{R}^d . We prove global well-posedness for the HFB equations for sufficiently regular pair interaction potentials, and establish key conservation laws. Moreover, we show that the solutions to the HFB equations exhibit a symplectic structure, and have a form reminiscent of a Hamiltonian system. In particular, this is used to relate the HFB equations to the HFB eigenvalue equations encountered in the physics literature. Furthermore, we construct the Gibbs states at positive temperature associated with the HFB equations, and establish criteria for the emergence of Bose-Einstein condensation.

1. INTRODUCTION

In this paper, we study the time-dependent generalization of the *Hartree-Fock-Bogoliubov (HFB) equations* which describe the quantum fluctuations of the Bose field around a Bose-Einstein condensate.

The starting point of our analysis is the evolution of the quantum many-body system of Bose particles with the quantum Hamiltonian

$$\mathbb{H} = \int dx \, \psi^*(x) h \psi(x) + \frac{1}{2} \int dx dy \, v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y), \quad (1)$$

with $h := -\Delta + V(x)$ acting on the variable x , defined on the scalar bosonic Fock space

$$\mathcal{F} := \bigoplus_{n \geq 0} (L^2(\mathbb{R}^d; \mathbb{C}))^{\otimes_{sym} n}, \quad (2)$$

where the n -th summand is an n -fold completely symmetric tensor product space, accounting for the Bose-Einstein statistics. Here, $\psi(x)$ and $\psi^*(x)$ stand for the annihilation and creation operators, respectively, satisfying the canonical commutation relations (CCR, see, e.g. [8]),

$$[\psi(x), \psi^*(y)] = \delta(x-y), \quad [\psi(x), \psi(y)] = 0 = [\psi^*(x), \psi^*(y)]. \quad (3)$$

For brevity, we write $\psi^\sharp(x)$ to denote either $\psi(x)$ or $\psi^*(x)$.

We assume that (a) the external potential V is infinitesimally form bounded with respect to the Laplacian $-\Delta$ and (b) $v^2 \leq C(1 - \Delta)$ in the sense of quadratic

forms, for some constant $C < \infty$. These conditions imply that \mathbb{H} is selfadjoint on the domain of the operator $\mathbb{H}_0 := \int dx \psi^*(x)(-\Delta)\psi(x)$ (see Appendix D).

States of our system are positive linear (‘expectation’) functionals ω on the Weyl CCR algebra \mathfrak{W} over Schwartz space $\mathcal{S}(\mathbb{R}^d)$. They can correspond either to non-zero densities and temperatures, or to a finite number of particles as in the case of BEC experiments in traps. In the latter case they are given by density operators on Fock space \mathcal{F} , $\omega(\mathbb{A}) = \text{Tr}(\mathbb{A}D)$, for all observables \mathbb{A} , where D is a positive, trace-class operator with unit trace on \mathcal{F} .

It is convenient to define states ω on products $\psi^\#(f_1) \dots \psi^\#(f_n)$ of creation and annihilation operators. This is done using derivatives ∂_{s_k} of expectation values $\omega(W(s_1 f_1) \dots W(s_n f_n))$ of the Weyl operators $W(f) := e^{i\phi(f)}$, with $\phi(f) := \psi^*(f) + \psi(f)$ (see [9], Section 5.2.3). We always assume that the states we consider are such that such derivatives (and therefore the corresponding correlation functions) exist, to arbitrary order. For $n \leq 4$, which is our case, this is guaranteed by assuming that $\omega(\mathbb{N}^2) < \infty$, where \mathbb{N} is the number operator $\mathbb{N} := \int dx \psi^*(x)\psi(x)$. This implies, in particular, that ω is given by a density operator.

As usual, it is convenient to pass from the multilinear functionals $\omega(\psi^\#(f_1) \dots \psi^\#(f_n))$ to the multi-variable functions $\omega(\psi^\#(x_1) \dots \psi^\#(x_n))$. Consequently, by an observable, we mean either an element of the Weyl algebra \mathfrak{W} or a linear combination of operators of the form $\psi^\#(f_1) \dots \psi^\#(f_n)$.

The evolution of states is given by the von Neumann-Landau equation ([31, 19], see also [33, 5] and, for some history, [37])

$$i\partial_t \omega_t(\mathbb{A}) = \omega_t([\mathbb{A}, \mathbb{H}]), \quad (4)$$

for all observables \mathbb{A} . We refer to [9, 25] for a mathematical justification of this equation.

1.1. Quasifree States and Truncated expectations. As the evolution (4) is extremely complicated, one is interested in manageable approximations. The natural and most commonly used approximation is given in terms of quasifree states, the simplest class of states.

Quasifree states are defined in terms of the truncated expectations with which we begin. We abbreviate $\psi_j := \psi^{\#j}(x_j)$. The (n^{th} order) *truncated expectations* (*correlation functions*) $\omega^T(\psi_1, \dots, \psi_n)$ of a state ω are defined recursively through

$$\omega(\psi_1 \dots \psi_n) = \sum_{P_n} \prod_{J \in P_n} \omega^T(\psi_{i_1}, \dots, \psi_{i_{\#(J)}}) \quad (5)$$

where P_n are partitions of the ordered set $\{1, \dots, n\}$ into ordered subsets, J . Thus, we have for example

$$\begin{aligned} \omega^T(\psi(x)) &= \omega(\psi(x)), \\ \omega^T(\psi_1, \psi_2) &= \omega(\psi_1 \psi_2) - \omega(\psi_1) \omega(\psi_2). \end{aligned} \quad (6)$$

A state ω is called *quasifree* if the truncated expectations $\omega^T(\psi_1, \dots, \psi_n)$ vanish for all $n > 2$. We denote quasifree states by ω^q and the set of quasifree states, by $\mathfrak{Q} \subseteq \mathfrak{S}$.

For quasifree states, all expectations $\omega^q(\psi_1^{\#1} \cdots \psi_n^{\#n})$, with $n > 2$, can therefore be expressed through $\omega^q(\psi_i^{\#i})$ and $\omega^q(\psi_j^{\#j} \psi_k^{\#k})$, with $i, j, k \in \{1, \dots, n\}$. The explicit formula is called *Wick's formula* or *Wick's theorem*, see [8]. Examples for small orders are given in Appendix A.

1.2. Quasifree reduction of the full dynamics. As was mentioned above, the detailed properties of the dynamics of the many-body system described by (4) are rather complicated, and an approximation is required to extract some key qualitative features. The main idea is to restrict the dynamics to quasifree states.

However, the property of being quasifree is not preserved by the dynamics given by (4) and the main question here is how to project the true quantum evolution onto the class of quasifree states.

The projection (or reduction) we propose is to map the solution ω_t of (4), with a quasifree initial state $\omega_0 \in \mathfrak{Q}$, to the family $(\omega_t^q)_{t \geq 0} \in C^1(\mathbb{R}_0^+; \mathfrak{Q})$ of quasifree states satisfying

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]) \quad (7)$$

for all observables \mathbb{A} , which are at most quadratic in the creation and annihilation operators. (For the Hamiltonian \mathbb{H} given by (1), the commutator $[\mathbb{A}, \mathbb{H}]$ contains products of at most 4 creation and annihilation operators.) This is the *quasifree reduction* of equation (4).

As was mentioned above, a quasifree state ω^q determines and is determined by the truncated expectations to the second order:

$$\begin{cases} \phi(x) := \omega^q(\psi(x)), \\ \gamma(x; y) := \omega^q[\psi^*(y) \psi(x)] - \omega^q[\psi^*(y)] \omega^q[\psi(x)], \\ \sigma(x, y) := \omega^q[\psi(x) \psi(y)] - \omega^q[\psi(x)] \omega^q[\psi(y)]. \end{cases} \quad (8)$$

Let γ and σ denote the operators with the integral kernels $\gamma(x, y)$ and $\sigma(x, y)$. This definition implies that

$$\gamma = \gamma^* \geq 0 \quad \text{and} \quad \sigma^* = \bar{\sigma}, \quad (9)$$

where $\bar{\sigma} = C\sigma C$ with C being the complex conjugation. (More detailed characterizations of γ and σ are given in Proposition 3.1.)

Evaluating (7) for monomials $\mathbb{A} \in \mathcal{A}^{(2)}$, where

$$\mathcal{A}^{(2)} := \{\psi(x), \psi^*(x)\psi(y), \psi(x)\psi(y)\},$$

yields a system of coupled nonlinear PDE's for $(\phi_t, \gamma_t, \sigma_t)$, the *Hartree-Fock-Bogoliubov (HFB) equations*. Since quasifree states are characterized by their truncated expectations ϕ, γ, σ , this system of equations is equivalent to equation (7).

To give a flavor of the HFB equations at this point, we formally assume the pair interaction potential to be a delta distribution, $v(x) = g\delta(x)$ with coupling

constant $g \geq 0$. The HFB equations then have the form

$$i\partial_t \phi_t = h_{g\delta}(\gamma_t^{\phi_t})\phi_t + gd(\sigma_t^{\phi_t})\bar{\phi}_t - 2g|\phi_t|^2\phi_t, \quad (10)$$

$$i\partial_t \gamma_t = [h_{g\delta}(\gamma_t^{\phi_t}), \gamma_t] + gd(\sigma_t^{\phi_t})\sigma_t^* - g\sigma_t \overline{d(\sigma_t^{\phi_t})}, \quad (11)$$

$$i\partial_t \sigma_t = [h_{g\delta}(\gamma_t^{\phi_t}), \sigma_t]_+ + g[d(\sigma_t^{\phi_t}), \gamma_t]_+ + d(\sigma_t^{\phi_t}), \quad (12)$$

where $[A, B]_+ = AB^T + BA^T$, $A^T := CA^*C$ and $d(\sigma)(x) := \sigma(x, x)$ and

$$\sigma^\phi := \sigma + \phi \otimes \phi, \gamma^\phi := \gamma + |\phi\rangle\langle\phi|, \quad (13)$$

$$h_{g\delta}(\gamma) := h + 2gd(\gamma). \quad (14)$$

Here and in what follows, we denote the *multiplication operators* and the *functions* by which they multiply by the *same symbols*. The difference is always clear from context.

The physical interpretation of the truncated expectations of ω_t^q is that ϕ_t gives the quantum mechanical wave function for the Bose-Einstein condensate, while γ_t and σ_t describe the dynamics of sound waves in the quasifree approximation (in particular, γ_t gives the density of the thermal cloud of atoms). (In the physics literature, $n = d(\gamma)$ and $m = d(\sigma)$ are called the non-condensate density and “anomalous” density, respectively.)

The HFB equations provide a *time-dependent extension* of the standard stationary Hartree-Fock-Bogoliubov equations for a Bose gas appearing in the physics literature, see e.g. [14, 15, 32]. Related equations (with $\phi_t = 0$) appear in superconductivity (Bogoliubov-de Gennes equations), where they are equivalent to the BCS effective Hamiltonian description.

1.3. Main Results. The quasifree reduction of the dynamics (4) and evaluation of the resulting equations for the truncated expectations ϕ, γ, σ – the HFB equations – are among the main results of this paper (see Theorem 2.2).

We show that the HFB equations are equivalent to the self-consistent equation

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{\text{hfb}}(\omega_t^q)]) \quad (15)$$

where $\mathbb{H}_{\text{hfb}}(\omega^q)$ is an explicitly constructed quadratic Hamiltonian (see (31)), for all observables \mathbb{A} . See Theorem 2.4.

Equation (15) suggests to define the *HFB stationary states* as the quasifree states satisfying

$$\omega^q([\mathbb{A}, \mathbb{H}_{\text{hfb}}(\omega^q)]) = 0,$$

for all observables \mathbb{A} . (If ω^q is given by a density matrix, we can rewrite this equation as a fixed point problem, see (16) below.) The most interesting among such states are the ground or Gibbs states. These states are defined as

$$\omega_{\beta, \mu}^q := \lim_{L \rightarrow \infty} \omega_L^q,$$

where ω_L^q is the quasifree ground or Gibbs state of the Bose gas confined to a torus, $\Lambda_L = \mathbb{R}^d/2L\mathbb{Z}^d$, i.e., the box $[-L, L]^d$, with periodic boundary conditions. It satisfies the fixed point equation

$$\Phi(\omega_L^q) = \omega_L^q \quad \text{with} \quad \Phi(\omega_L^q)(\mathbb{A}) := \text{Tr}[\mathbb{A} \exp(-\beta(\mathbb{H}_{\text{hfb}}(\omega_L^q) - \mu\mathbb{N}))/\Xi] \quad (16)$$

where $\beta > 0$ is the inverse temperature, μ is the chemical potential, and $\Xi = \text{Tr}[\exp(-\beta(\mathbb{H}_{hfb}(\omega_L^q) - \mu\mathbb{N})) - \mu\mathbb{N}]$, and is a stationary solution to the equation (15) on Λ_L . (To prove the second statement, $\omega^q([\mathbb{H}_{hfb}(\omega^q), \mathbb{A}]) := \lim_{L \rightarrow \infty} \omega_L^q([\mathbb{H}_{hfb}(\omega^q), \mathbb{A}]) = 0$, for any observable \mathbb{A} defined on some torus Λ_L .)

We also initiate a mathematical discussion of the HFB equations. In particular, for γ trace-class and σ Hilbert-Schmidt operators (for the precise restriction see Section 2), we show

- Global well-posedness (Theorem 5.1) of the HFB equations;
- Conservation of the total particle number

$$\mathcal{N}(\phi_t, \gamma_t, \sigma_t) := \omega_t^q(\mathbb{N}), \quad (17)$$

where \mathbb{N} is the number operator (see Corollary 2.7);

- Existence and conservation (under certain conditions on v and ω_t^q) of the energy:

$$\mathcal{E}(\phi_t, \gamma_t, \sigma_t) := \omega_t^q(\mathbb{H}) \quad (18)$$

(see Corollary 2.7 and Theorem 2.8, or Prop 3.12).

More generally, any observable conserved by the von Neumann-Landau dynamics and which is at most quadratic in the creation and annihilation operators is also conserved by the quasifree dynamics. See Theorem 2.5. In the special case of the observable \mathbb{N} , this gives the statement above.

Note that conservation of the total particle number is related to the $U(1)$ -gauge invariance, i.e., invariance under the transformation $\psi^\# \rightarrow (e^{i\theta}\psi)^\#$, of the Hamiltonian \mathbb{H} .

The total particle number and energy, $\mathcal{N}(\phi, \gamma, \sigma) := \omega^q(\mathbb{N})$ and $\mathcal{E}(\phi, \gamma, \sigma) := \omega^q(\mathbb{H})$, as functions of (ϕ, γ, σ) can be evaluated explicitly:

$$\mathcal{N}(\phi, \gamma, \sigma) = \int (\gamma(x; x) + |\phi(x)|^2) dx, \quad (19)$$

and, in the case of a delta pair potential $v = g\delta$, the energy, $\mathcal{E}(\phi, \gamma, \sigma)$, takes the form

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) = & \text{Tr}[h(\gamma + |\phi\rangle\langle\phi|)] \\ & + g \int (2n(x)|\phi(x)|^2 + n(x)^2 + \frac{1}{2}|w(x)|^2) dx. \end{aligned} \quad (20)$$

(In terms of $\mathbb{H}_{hfb}(\omega^q)$, we have that $\mathcal{E}(\phi, \gamma, \sigma) := \omega^q(\mathbb{H}) = \omega^q(\mathbb{H}_{hfb}(\omega^q)) + \text{scalar}$.)

As usual, for γ trace class and σ Hilbert-Schmidt, the energy provides the variational characterization of stationary Gibbs states:

- Gibbs states minimize the energy $\mathcal{E}(\phi, \gamma, \sigma)$ under the constraint of constant entropy and the expected number of particles.

In the thermodynamic limit, with $V = 0$, one should replace the energy and the number of particles by the energy and particle number densities.

Quasifree states ω^q that are $U(1)$ -gauge invariant, i.e. which satisfy $\omega^q(\psi) = \omega^q(e^{i\theta}\psi), \forall \theta$, etc, have vanishing truncated expectations ϕ_{ω^q} and σ_{ω^q} . Indeed, the $U(1)$ -gauge invariance of ω^q implies that $\omega^q(\psi) = \omega^q(e^{i\theta}\psi) = e^{i\theta}\omega^q(\psi)$, which yields $\phi_{\omega^q} = 0$. Similarly one shows that $\sigma_{\omega^q} = 0$. For quasifree, $U(1)$ -gauge invariant states, the HFB equations reduce to the bosonic Hartree-Fock equation.

For $V = 0$ and γ and σ translationally invariant, our full energy functional (see (35)) reduces to the energy density functional going back to the work [13] and considered in [28, 29]. It is shown in the latter papers that this functional has minimizers under the constraint of constant entropy and particle densities. [28, 29] show also the appearance of a Bogoliubov condensate for the corresponding minimizers. (One still has to show that states thus obtained are stationary solutions to the equation (15).)

In this paper we do not consider the general problem of existence of static solutions. However, for $V = 0$, we present a result on the existence of the positive temperature, $U(1)$ -gauge and translation invariant Gibbs HFB states and show that Bose-Einstein condensation (BEC) occurs above a critical density, see Theorem 6.3.

As was mentioned above, the $U(1)$ -gauge invariant states have $\phi = 0$ and $\sigma = 0$ and therefore are, in fact, stationary solutions of the bosonic Hartree-Fock equation. Moreover, as the results of [28, 29] show, in the BEC regime, these states are not minimizers of the full HFB (mean) energy for the (mean) entropy and number of particles fixed. However, the existence of such states exhibiting Bose-Einstein condensation indicates that there are also symmetry breaking Gibbs HFB states, i.e. with $\phi \neq 0$ and $\sigma \neq 0$.

1.4. Fixed Point Equation. Let $\mathbb{U}_{\omega^q}(t, s)$ denote the unitary propagator on the Fock space solving

$$\begin{aligned} i\partial_t \mathbb{U}_{\omega^q}(t, s) &= \mathbb{H}_{hfb}(\omega_t^q) \mathbb{U}_{\omega^q}(t, s), \\ \mathbb{U}_{\omega^q}(s, s) &= \mathbf{1}. \end{aligned} \tag{21}$$

Then, we can rewrite the equation (15) with an initial condition ω_0^q as an ‘integral’ equation

$$\omega_t^q(\mathbb{A}) = \omega_0^q(\mathbb{U}_{\omega^q}(t, 0)^* \mathbb{A} \mathbb{U}_{\omega^q}(t, 0)), \tag{22}$$

where \mathbb{A} is an arbitrary observable. This is the fixed point problem, $\omega_t^q = \Phi(\omega_t^q)$, where $\Phi(\omega_t^q)(\mathbb{A}) := \omega_0^q(\mathbb{U}_{\omega^q}(t, 0)^* \mathbb{A} \mathbb{U}_{\omega^q}(t, 0))$. Since $\mathbb{U}_{\omega^q}(t, s)$ are generated by quadratic Hamiltonians, we have that $\omega_0^q(\mathbb{U}_{\omega^q}(t, 0)^* \mathbb{A} \mathbb{U}_{\omega^q}(t, 0))$ is quasifree for any time $t > 0$. This formulation opens an opportunity to proving the existence of the quasifree dynamics directly, without going to the truncated expectations.

In this article, we do not show that the HFB equations provide an accurate approximation of the many-body dynamics (4) for finite times. There is a considerable literature on the derivation of the simpler Hartree and Hartree – Fock equations. Recently, the Hartree equation with linear fluctuations around the Hartree solutions (producing the linearized HFB equations with respect to γ and σ) were derived in [16, 23, 26, 22, 21], see [20] for a recent review.

1.5. Organization of the paper. In Section 2, we present the HFB equations, which we prove in Appendix B using the method of quasifree reduction, applied to the interacting Bose field in \mathbb{R}^d characterized by the Hamiltonian (1). We also show that conservation laws for the many-body problem imply conservation laws for the HFB equation. In Section 3, we show that the solutions to the HFB equations possess a symplectic structure, and that they have similarities with a Hamiltonian system. In Section 4 we show how the symplectic version of the HFB equations and the HFB eigenvalue equations found in the physics literature are related. In Section 5, we prove that the Cauchy problem for the HFB equations is globally well-posed in the energy space, provided that the pair interaction potential is sufficiently regular.

Our proof of global well-posedness is in part inspired by previous works on the Hartree-Fock equation [6, 12, 7, 11, 38]. In Section 6, we give a proof of the Bose-Einstein condensation in the stationary case. A brief account on quasifree states along with the proofs of various technical lemmata are collected in the Appendices.

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2. THE HFB EQUATIONS AND THEIR BASIC PROPERTIES

In this section, we formulate the HFB equations for a general pair potential v and prove the associated conservation laws. The derivation of the HFB equations is done in Appendix B by applying the quasifree reduction as in the introduction.

Notations. Let $M := \langle \nabla_x \rangle = \sqrt{1 - \Delta_x}$, with Δ_x being the Laplacian in d dimensions. We denote by \mathcal{B} the space of bounded operators on $L^2(\mathbb{R}^d)$, with the operator norm denoted by $\|\cdot\|$. For $j \in \mathbb{N}_0$ we define the spaces

$$X^{j,\infty} = \{(\phi, \gamma, \sigma) \in H^j \times \mathcal{B}^j \times \mathcal{B}^j : \gamma = \gamma^* \geq 0 \text{ and } \sigma^* = \bar{\sigma}\}, \quad (23)$$

with H^j the Sobolev space $H^j(\mathbb{R}^d)$ and $\mathcal{B}^j = M^{-j}\mathcal{B}M^{-j}$. The norms on $X^{j,\infty}$ are given by the norms on the Banach spaces, $H^j \times \mathcal{B}^j \times \mathcal{B}^j$, i.e.,

$$\|(\phi, \gamma, \sigma)\|_{X^{j,\infty}} = \|M^j \phi\|_{L^2(\mathbb{R}^d)} + \|M^j \gamma M^j\| + \|M^j \sigma M^j\|.$$

(The superindex ∞ indicates that we are dealing with bounded operators, as opposed to the trace-class and Hilbert-Schmidt ones appearing later.)

Moreover, we let $\mathcal{X}_T^\infty := C^0([0, T]; X^{j,\infty}) \cap C^1([0, T]; X^{0,\infty})$, for a fixed j satisfying $j > d/2$ and $j \geq 2$, and denote by $X_{\text{qf}}^{j,\infty}$ and $\mathcal{X}_{T,\text{qf}}^\infty$ spaces of quasifree states and families of quasifree states with the 1st and 2nd order truncated expectations from the spaces $X^{j,\infty}$ and \mathcal{X}_T^∞ , respectively.

The reason for introducing the spaces \mathcal{B}^j is the following elementary result.

Lemma 2.1. *Any $\alpha \in \mathcal{B}^j, j > d/2$, has a bounded, Hölder continuous integral kernel $\alpha(x, y)$.*

Let $v \in L^1$. Then the operator $k : \alpha \rightarrow v \sharp \alpha$, defined through its integral kernel:

$$v \sharp \alpha(x; y) := v(x - y)\alpha(x; y), \quad (24)$$

is bounded from $\mathcal{B}^j, j > d/2$, to $\mathcal{B}^s, s < j - d/2$.

Proof. Let $G(x)$ be the Fourier transform of the function $(1 + |\xi|^2)^{-j/2}, j > d/2$. Then $G \in H^s(\mathbb{R}^d), s < j - d/2$, and we can write $\alpha(x, y) = \langle G_x, \alpha_1 G_y \rangle$, where $G_x(x') := G(x - x')$ and $\alpha_1 := M^j \alpha M^j$. Since $\alpha \in \mathcal{B}^j, j > d/2$, α_1 is a bounded operator and therefore $|\alpha(x, y)| \leq \|G_x\|_{L^2} \|\alpha_1\| \|G_y\|_{L^2} = \|\alpha_1\| \|G\|_{L^2}^2$. Similarly, one shows the Hölder continuity.

For the second statement, the result above gives $\|(v \sharp \alpha)f\|_{L^2} \leq \|\alpha(\cdot)\|_{L^\infty} \|v\| * \|f\|_{L^2} \leq \|\alpha(\cdot)\|_{L^\infty} \|v\|_{L^1} \|f\|_{L^2}$. Similarly, one shows the estimates involving M^s . \square

In what follows we use the *same notation for functions and the operators of multiplication by these functions*. Which one is meant in every instance is clear from the context.

Theorem 2.2. *Assume that the pair interaction potential v is even, $v(x) = v(-x)$, infinitesimally Δ -bounded, with $v \in L^1(\mathbb{R}^d)$. Then $\omega_t^q \in \mathcal{X}_{T, \text{qf}}^\infty$ satisfies*

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]), \quad \forall \mathbb{A} \in \mathcal{A}^{(2)}, \quad (25)$$

with the Hamiltonian \mathbb{H} defined in (1), if and only if the triple $(\phi_t, \gamma_t, \sigma_t) \in \mathcal{X}_T^\infty$ of the 1st and 2nd order truncated expectations of ω_t^q satisfies the time-dependent Hartree-Fock-Bogoliubov equations

$$i\partial_t \phi_t = h(\gamma_t)\phi_t + k(\sigma_t^{\phi_t})\bar{\phi}_t, \quad (26)$$

$$i\partial_t \gamma_t = [h(\gamma_t^{\phi_t}), \gamma_t] + k(\sigma_t^{\phi_t})\sigma_t^* - \sigma_t k(\sigma_t^{\phi_t})^*, \quad (27)$$

$$i\partial_t \sigma_t = [h(\gamma_t^{\phi_t}), \sigma_t]_+ + [k(\sigma_t^{\phi_t}), \gamma_t]_+ + k(\sigma_t^{\phi_t}), \quad (28)$$

where $[A_1, A_2]_+ = A_1 A_2^T + A_2 A_1^T$, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + |\phi\rangle\langle\phi|$, and

$$h(\gamma) = h + b[\gamma], \quad b[\gamma] := v * d(\gamma) + v \sharp \gamma, \quad (29)$$

$$k(\sigma) = v \sharp \sigma, \quad d(\alpha)(x) := \alpha(x, x). \quad (30)$$

If $v = g\delta$, $h(\gamma)$ agrees with $h_{g\delta}(\gamma)$ in (13), and $k(\sigma)$ agrees with the multiplication operator by $g d(\sigma)(x)$ in (13).

Due to Lemma 2.1 and the fact that $h(\gamma_t)$ is Δ -bounded, for each $t > 0$, the r.h.s. of (26) - (28) belongs to the space $X^{0, \infty}$. The proof of Theorem 2.2 is given in Appendix B.

Remark 2.3. *If we base our spaces for γ and σ on the trace-class and Hilbert-Schmidt operators, instead of bounded ones, then we can relax the conditions on the potentials.*

We now show that equations (7) (or (26) to (28)) and (15) describing the quasifree dynamics are equivalent.

For a quasifree state ω^q with 1^{st} and 2^{nd} order truncated expectations $(\phi, \gamma, \sigma) \in X^1$, we define the quadratic Hamiltonian parametrized by (ϕ, γ, σ) as

$$\begin{aligned} \mathbb{H}_{hfb}(\omega^q) &= \int \psi^*(x) h_v(\gamma) \psi(x) dx \\ &\quad - \int b[|\phi\rangle\langle\phi|] \phi(x) \psi^*(x) dx + h.c. \\ &\quad + \frac{1}{2} \int \psi^*(x) (v \# \sigma) \psi^*(x) dx + h.c.. \end{aligned} \quad (31)$$

Theorem 2.4. *Assume that the pair potential v is even, $v(x) = v(-x)$, and satisfies $v^2 \leq CM^2$ for some $C > 0$. Then $(\phi_t, \gamma_t, \sigma_t) \in \mathcal{X}_T^\infty$ satisfy the HFB equations (26) to (28) if and only if the corresponding quasifree state $\omega_t^q \in \mathcal{X}_{T,qf}^\infty$ satisfies the equation*

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{hfb}(\omega_t^q)]) . \quad (32)$$

The proof of Theorem 2.4 is given in Appendix C.

We now prove the conservation laws for the number of particles (or more generally, for any observable commuting with the Hamiltonian \mathbb{H} which is quadratic with respect to creation and annihilation operators), and for the energy.

Theorem 2.5. *Assume that an observable $\mathbb{A} \in \mathcal{A}^{(2)}$ satisfies $[\mathbb{H}, \mathbb{A}] = 0$. Then $\omega_t^q(\mathbb{A})$ is conserved:*

$$\omega_t^q(\mathbb{A}) = \omega_0^q(\mathbb{A}) \quad \forall t \in \mathbb{R} . \quad (33)$$

Proof. This follows from (25) for \mathbb{A} of order up to two, with $[\mathbb{A}, \mathbb{H}] = 0$. \square

To draw some consequences from this result we need to define additional spaces.

Remark 2.6. *We identify Hilbert-Schmidt operators on $L^2(\mathbb{R}^d)$, denoted by \mathcal{L}^2 , with their kernels in $L^2(\mathbb{R}^{2d})$, if no confusion may arise.*

Notations. We denote by \mathcal{L}^1 the space of trace-class operators on $L^2(\mathbb{R}^d)$ endowed with the trace norm $\|\cdot\|_{\mathcal{L}^1}$. For $j \in \mathbb{N}_0$ we define the spaces

$$X^j = \{(\phi, \gamma, \sigma) \in H^j \times \mathcal{H}^j \times H_s^j\} , \quad (34)$$

with H^j being the Sobolev space $H^j(\mathbb{R}^d)$, $\mathcal{H}^j = M^{-j} \mathcal{L}^1 M^{-j}$, and H_s^j the Sobolev space $H^j(\mathbb{R}^{2d})$ restricted to functions σ such that $\sigma(x, y) = \sigma(y, x)$. These are real Banach spaces, similar to the Sobolev spaces $H^j(\mathbb{R}^d)$ in the scalar case, when endowed with the norms

$$\|(\phi, \gamma, \sigma)\|_{X^j} = \|M^j \phi\|_{L^2(\mathbb{R}^d)} + \|M^j \gamma M^j\|_{\mathcal{L}^1} + \|(M^2 \otimes 1 + 1 \otimes M^2)^{j/2} \sigma\|_{L^2(\mathbb{R}^{2d})} .$$

The norm $\|(M^2 \otimes 1 + 1 \otimes M^2)^{j/2} \sigma\|_{L^2(\mathbb{R}^{2d})}$ is equivalent to the usual $\|\sigma\|_{H^j(\mathbb{R}^{2d})}$ norm.

Furthermore, we let $\mathcal{X}_T := C^0([0, T]; X^3) \cap C^1([0, T]; X^1)$ and, as above, we denote by X_{qf}^j and \mathcal{X}_T^{qf} the spaces of quasifree states and families of quasifree

states with the 1^{st} and 2^{nd} order truncated expectations from the spaces X^j and \mathcal{X}_T , respectively.

Corollary 2.7. *Let $\omega_t^q \in \mathcal{X}_T^{qf}$ solve (25) (or (32)). Then the number of particles $\mathcal{N}(\phi_t, \gamma_t, \sigma_t) = \omega_t^q(\mathbb{N})$ is conserved.*

If, in addition, v is as in Theorem 2.4, then the energy $\omega_t^q(\mathbb{H})$ is conserved.

Theorem 2.8. *Let v be as in Theorem 2.4 and $\omega^q \in X^{qf}$. Then the energy $\omega^q(\mathbb{H}) = \mathcal{E}(\phi, \gamma, \sigma)$ is given explicitly as*

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \text{Tr}[h(\gamma + |\phi\rangle\langle\phi|)] + \text{Tr}[b[|\phi\rangle\langle\phi|]\gamma] \\ &\quad + \frac{1}{2}\text{Tr}[b[\gamma]\gamma] + \frac{1}{2} \int v(x-y)|\sigma(x, y) + \phi(x)\phi(y)|^2 dx dy. \end{aligned} \quad (35)$$

Proof. We use

$$\omega_C^q(\mathbb{A}) := \omega^q(W_\phi \mathbb{A} W_\phi^*), \quad (36)$$

where the Weyl operators are defined through $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$ and satisfy

$$W_\phi^* \psi(x) W_\phi = \psi(x) + \phi(x). \quad (37)$$

Note that the state $\omega_{C,t}^q$ is quasifree because ω^q is quasifree. By construction $\omega_C^q(\psi(x)) = 0$ and thus using (5) and the quasifreeness of ω_C^q one sees that ω_C^q vanishes on monomials of odd order in the creation and annihilation operators. Note that $\mathcal{E}(\phi, \gamma, \sigma) = \omega_C^q(W_\phi^* \mathbb{H} W_\phi)$, hence using the vanishing on monomials of odd order in the creation and annihilation operators

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \omega_{C,t}^q \left(\int v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) dx dy \right. \\ &\quad + \frac{1}{2} \left(\int v(x-y) \phi_t(x) \phi_t(y) \psi^*(x) \psi^*(y) dx dy + h.c. \right) \\ &\quad + \int (h + b[|\phi\rangle\langle\phi|])(x; y) \psi^*(x) \psi(y) dx dy \\ &\quad \left. + \frac{1}{2} \int |\phi(x)\phi(y)|^2 v(x-y) dx dy + \langle \phi, h\phi \rangle \right). \end{aligned}$$

Then, using that ω_C^q is a quasifree state with expectations $(0, \gamma, \sigma)$ yields

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \frac{1}{2} \text{Tr}[b[\gamma]\gamma] + \frac{1}{2} \int \overline{\sigma(x, y)} v(x-y) \sigma(x, y) dx dy \\ &\quad + \Re \left(\int \overline{\sigma(x, y)} v(x-y) \phi(x) \phi(y) dx dy \right) \\ &\quad + \text{Tr}[(h + b[|\phi\rangle\langle\phi|])\gamma] + \frac{1}{2} \int |\phi(x)\phi(y)|^2 v(x-y) dx dy + \langle \phi, h\phi \rangle \end{aligned}$$

which gives the expression of the energy in terms of ϕ , γ and σ . \square

3. GENERALIZED ONE-PARTICLE DENSITY MATRIX AND BOGOLUBOV TRANSFORMS

In this section, we consider the HFB equations (27) - (28) for γ_t and σ_t and reformulate them in terms the generalized one-particle density matrix $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \sigma_t^* & 1 + \gamma_t \end{pmatrix}$.

We show that the diagonalizing maps for Γ_t are symplectomorphisms (see below for the definition) and that the resulting equation for Γ_t is equivalent to the evolution equation for these symplectomorphisms. The latter will allow us to (a) give another proof of the conservation of energy without using the second quantization framework and (b) connect the time-dependent HFB equations (27) - (28) to the time-independent HFB equations used in the physics literature. See Section 4.

We begin by relating properties of $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix}$ to those of γ and σ .

Proposition 3.1. *The generalized one-particle density matrix, Γ , satisfies:*

$$\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0. \quad (38)$$

This property is equivalent to the following statements:

- (1) *The operator $\gamma \geq 0$ is positive semidefinite.*
- (2) *The expectation $\sigma(x, y) = \sigma(y, x)$ is symmetric.*
- (3) *The inequality $\sigma(1 + \bar{\gamma})^{-1} \sigma^* \leq \gamma$ holds.*
- (4) *The bound $\frac{1}{2} \|\sigma\|_{H_s^1}^2 \leq \|\gamma\|_{\mathcal{H}^1} (1 + \text{Tr}[\gamma])$ holds.*

(Statement (4) follows from (1) and (3) and is given here for later convenience of references.)

Proof. We remark that the truncated expectations γ and σ are the expectations of the state

$$\omega_C(\mathbb{A}) := \omega(W_{\phi_t} \mathbb{A} W_{\phi_t}^*)$$

where $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$ are the Weyl operators. W_ϕ satisfy $W_\phi \psi(x) W_\phi^* = \psi(x) - \phi(x)$. The generalized one particle density matrix Γ of ω_C is non-negative, since, for all f, g in L^2 ,

$$\left\langle \begin{pmatrix} f \\ g \end{pmatrix}, \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \right\rangle = \omega_C((\psi^*(f) + \psi(\bar{g}))(\psi(f) + \psi^*(\bar{g}))) \geq 0. \quad (39)$$

Statements (1) and (2) are obvious. The inequality in Point (3) follows from the Schur complement argument:

$$\begin{aligned} 0 &\leq \begin{pmatrix} 1 & -\sigma(1 + \bar{\gamma})^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma & \sigma \\ \sigma^* & 1 + \bar{\gamma} \end{pmatrix} \begin{pmatrix} 1 & -\sigma(1 + \bar{\gamma})^{-1} \\ 0 & 1 \end{pmatrix}^* \\ &= \begin{pmatrix} \gamma - \sigma(1 + \bar{\gamma})^{-1} \sigma^* & 0 \\ 0 & 1 + \bar{\gamma} \end{pmatrix}. \end{aligned}$$

Finally, we observe that (1) and (3) and the inequality $\gamma \leq \text{Tr}[\gamma] \mathbf{1}$ imply the following bound on $\sigma \sigma^*$,

$$(1 + \text{Tr}[\gamma])^{-1} \sigma \sigma^* \leq \sigma(1 + \bar{\gamma})^{-1} \sigma^* \leq \gamma.$$

Inserting $M = \sqrt{1 - \Delta_x}$ on both sides and taking the trace yields (4). \square

Notations. For $j \in \mathbb{N}_0$ we define the spaces

$$Y^j = \mathcal{H}^j \times H_s^j, \quad (40)$$

where the spaces \mathcal{H}^j and H_s^j are defined after (34). The norms on Y^j are given by

$$\|(\gamma, \sigma)\|_{Y^j} = \|\gamma\|_{\mathcal{H}^j} + \|\sigma\|_{H_s^j},$$

where $\|\gamma\|_{\mathcal{H}^j} := \|M^j \gamma M^j\|_{\mathcal{L}^1(L^2(\mathbb{R}^d))}$ and $\|\sigma\|_{H_s^j} := \|(M^2 \otimes 1 + 1 \otimes M^2)^{j/2} \sigma\|_{L^2(\mathbb{R}^{2d})}$. We also use the spaces $\mathcal{Y}_T := C^0([0, T]; Y^3) \cap C^1([0, T]; Y^1)$ and $\tilde{\mathcal{Y}}_T :=$ the space of generalized one-particle density matrices, Γ , with entries in \mathcal{Y}_T .

In what follows we fix a number $T > 0$ and a family $\phi_t \in C^0([0, T]; H^3) \cap C^1([0, T]; H^1)$ (not necessarily a solution (26)) and do not display it in our notation. A simple computation yields the first result of this section:

Proposition 3.2. $(\gamma_t, \sigma_t) \in \mathcal{Y}_T$ is a solution to the HFB equations (27) - (28) iff $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \sigma_t^* & 1 + \bar{\gamma}_t \end{pmatrix} \in \tilde{\mathcal{Y}}_T$ solves the equation

$$i\partial_t \Gamma_t = \mathcal{S} \Lambda(\Gamma_t) \Gamma_t - \Gamma_t \Lambda(\Gamma_t) \mathcal{S}, \quad (41)$$

with $\Lambda(\Gamma) = \begin{pmatrix} h(\gamma) & k(\sigma) \\ k(\sigma)^* & h(\gamma) \end{pmatrix}$, where, recall, $h(\gamma)$ and $k(\sigma)$ are defined in (29) and (30), and $\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

To formulate the next result we introduce some definitions.

Definition 3.3. Let \mathfrak{h} denote a complex Hilbert space. A bounded linear operator $\mathcal{U} = \begin{pmatrix} u & v \\ v^* & \bar{u} \end{pmatrix}$ on $\mathfrak{h} \times \mathfrak{h}$ with the property that

$$\mathcal{U}^* \mathcal{S} \mathcal{U} = \mathcal{S} \quad \text{and} \quad \mathcal{U} \mathcal{S} \mathcal{U}^* = \mathcal{S}, \quad (42)$$

with $\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, is called a symplectomorphism.

If, moreover, there exists a unitary transformation \mathbb{U} on the Fock space, sometimes called implementation of \mathcal{U} , such that

$$\forall f, g \in \mathfrak{h}, \quad \mathbb{U}[\psi^*(f) + \psi(\bar{g})] \mathbb{U}^* = \psi^*(uf + vg) + \psi(v\bar{f} + u\bar{g}),$$

then the symplectomorphism \mathcal{U} is said to be implementable.

Remark 3.4. The operator \mathcal{U} is a symplectomorphism in the sense that it preserves the symplectic form $\Im\langle \cdot, \mathcal{S} \cdot \rangle$ on $\mathfrak{h} \times \mathfrak{h}$ (i.e. is a canonical map). (In fact, \mathcal{U} preserves $\langle \cdot, \mathcal{S} \cdot \rangle$.)

Remark 3.5. The operator \mathcal{U} is a symplectomorphism if and only if the operator $f \mapsto uf + v\bar{f}$ is a symplectomorphism on $(\mathfrak{h}, \Im\langle \cdot, \cdot \rangle)$ in the usual sense (i.e., it preserves the symplectic form $\Im\langle \cdot, \cdot \rangle$).

Remark 3.6. The conditions in (42) are equivalent to satisfying the four equations

$$uu^* - vv^* = \mathbf{1}, \quad u^*u - v^T \bar{v} = \mathbf{1}, \quad u^*v = v^T \bar{u}, \quad uv^T = vu^T. \quad (43)$$

Remark 3.7. The transformation

$$\forall f, g \in \mathfrak{h}, \quad (\psi^*(f), \psi(\bar{f})) \rightarrow (\psi^*(uf) + \psi(v\bar{f}), \psi^*(vf) + \psi(u\bar{f})) \quad (44)$$

is called the Bogoliubov transformation. It is easy to check that it preserves the CCR iff the operator $\mathcal{U} = \begin{pmatrix} u & v \\ v^* & \bar{u} \end{pmatrix}$ satisfies (42).

If v is Hilbert-Schmidt, then the Bogoliubov transformation (44) is implementable. This condition is referred to as the Shale condition; see [36].

For later use, we introduce the Banach space

$$\mathcal{H}^{\infty,2} = \left\{ \begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix} \mid a \in \mathcal{B}(H^1) \simeq M\mathcal{B}M^{-1}, \quad b \in M\mathcal{L}^2M^{-1} \right\},$$

endowed with the norm $\left\| \begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix} \right\|_{\mathcal{H}^{\infty,2}} = \|a\|_{\mathcal{B}(H^1)} + \|b\|_{M\mathcal{L}^2M^{-1}}$, using the same identification between operators and kernels as before.

We begin with an auxiliary result:

Proposition 3.8. *Let $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \sigma & 1+\bar{\gamma} \end{pmatrix} \in Y^1$ and $\Gamma \geq 0$. Then there exist an implementable symplectomorphism $\mathcal{U} \in \mathcal{H}^{\infty,2}$ such that*

$$\Gamma = \mathcal{U} \begin{pmatrix} \gamma' & 0 \\ 0 & 1 + \overline{\gamma'} \end{pmatrix} \mathcal{U}^*,$$

where $0 \leq \gamma' \leq \gamma$. The operator γ' is unique up to conjugation by a unitary operator.

This result is related to Theorem 1 of [27], which is stronger. See also [2, 3]. As the relation between the two results is not obvious, we give a direct proof of Proposition 3.8 after the proof of Proposition 3.9.

The next result relates the evolution of Γ_t to the evolution of implementable symplectomorphisms $\mathcal{U}_t \in \mathcal{H}^{\infty,2}(\mathfrak{h} \times \mathfrak{h})$, diagonalizing Γ_t .

Proposition 3.9. (i) *For any $\Gamma_t \in \tilde{\mathcal{Y}}_T$ and any implementable symplectomorphism $\mathcal{U}_0 \in \mathcal{H}^{\infty,2}$, the initial value problem*

$$i\partial_t \mathcal{U}_t^* = \mathcal{S}\Lambda(\Gamma_t)\mathcal{U}_t^*, \quad \mathcal{U}_{t=0} = \mathcal{U}_0, \quad (45)$$

has a unique solution in $\mathcal{H}^{\infty,2}$, which is a symplectomorphism for every t .

(ii) *Let $\Gamma_t \in \tilde{\mathcal{Y}}_T$ solve the equation (41), with an initial condition $\Gamma_0 \in \tilde{Y}^3$, s.t. $\Gamma_0 \geq 0$. Let \mathcal{U}_0 be an implementable symplectomorphism diagonalizing Γ_0 :*

$$\Gamma_0 = \mathcal{U}_0 \Gamma'_0 \mathcal{U}_0^*, \quad \Gamma'_0 = \begin{pmatrix} \gamma'_0 & 0 \\ 0 & 1 + \overline{\gamma'_0} \end{pmatrix}.$$

Then the continuous family of implementable symplectomorphisms \mathcal{U}_t in $\mathcal{H}^{\infty,2}(\mathfrak{h} \times \mathfrak{h})$ satisfying (45), with the above \mathcal{U}_0 , diagonalizes Γ_t :

$$\Gamma_t = \mathcal{U}_t^* \Gamma'_0 \mathcal{U}_t \geq 0. \quad (46)$$

Proof of Prop. 3.9. The operator Λ_t can be decomposed as $\Lambda_t = \Lambda_1 + \Lambda_{2,t}$ with

$$\Lambda_1 = \begin{pmatrix} h & 0 \\ 0 & \bar{h} \end{pmatrix}, \quad \Lambda_{2,t} = \begin{pmatrix} b[\gamma_t + |\phi_t\rangle\langle\phi_t|] & k[\sigma_t + \phi \otimes \phi] \\ k[\sigma_t + \phi \otimes \phi] & b[\gamma_t + |\phi_t\rangle\langle\phi_t|] \end{pmatrix}.$$

The first operator, Λ_1 , is the generator of a continuous one-parameter group in $\mathcal{H}^{\infty,2}$. As for the second one, using the continuity of $t \mapsto \rho_t \in X^1$, and Prop. E.1, we get the continuity of $t \mapsto \Lambda_{2,t} \in \mathcal{H}^{\infty,2}$. We can thus use classical results of functional analysis (see, e.g., [18]) to obtain the existence and uniqueness of \mathcal{U}_t and its regularity.

The same arguments as in the next lemma prove that \mathcal{U}_t is a symplectomorphism.

Finally, Γ_t and $\mathcal{U}_t^* \Gamma_0 \mathcal{U}_t$ satisfy the same differential equation, and the uniqueness of a solution to (45) proves the last equality. \square

Proof of existence in Prop. 3.8. We split the proof into two lemmas, Lemmas 3.10 and 3.11 below. The strategy is to construct Γ_t and symplectomorphisms \mathcal{U}_t such that $\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \Gamma_0$, for all t , and in the limit $t \rightarrow \infty$, Γ_∞ has the desired form. The key step will be to use a differential equation for Γ_t implying $\|\sigma_t\|_{H_s^1} \searrow 0$.

Lemma 3.10. *Let $T > 0$ and $\Lambda_t = \begin{pmatrix} a_t & b_t \\ \bar{b}_t & \bar{a}_t \end{pmatrix} \in C([0, T]; \mathcal{H}^{\infty, 2})$. Then, the ordinary differential equation*

$$i\partial_t \mathcal{U}_t^* = S \Lambda_t \mathcal{U}_t^*, \quad (47)$$

with initial data $\mathcal{U}_0^ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, has a unique global solution $\mathcal{U}_t \in C^1([0, T]; \mathcal{H}^{\infty, 2})$, and \mathcal{U}_t is a symplectomorphism for all time.*

Moreover, if $\gamma_t \in C^1([0, T]; \mathcal{H}^1)$, $\sigma_t \in C^1([0, T]; H_s^1)$ satisfy

$$i\partial_t \gamma_t = a_t \gamma_t - b_t \bar{\sigma}_t - \gamma_t a_t + \sigma_t \bar{b}_t, \quad (48)$$

$$i\partial_t \sigma_t = a_t \sigma_t - b_t(1 + \bar{\gamma}_t) - \gamma_t b_t + \sigma_t \bar{a}_t, \quad (49)$$

with initial data $\sigma_0 = \sigma$, $\gamma_0 = \gamma$ given in Prop 3.9(i), then, for all time t ,

$$\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \Gamma_0. \quad (50)$$

Proof. The existence and uniqueness of \mathcal{U}_t^* follows from the theory of time-dependent linear ordinary differential equations once one observes that \mathcal{H}^1 and H_s^1 are continuously embedded in $\mathcal{B}(H^1)$ and $M\mathcal{L}^2(L^2)M^{-1}$. At $t = 0$, $\mathcal{U}_0 S \mathcal{U}_0^* = \mathcal{S}$ and

$$i\partial_t (\mathcal{U}_t S \mathcal{U}_t^*) = \mathcal{U}_t (-\Lambda_t S S + S S \Lambda_t) \mathcal{U}_t^* = 0,$$

thus $\mathcal{U}_t S \mathcal{U}_t^* = \mathcal{S}$ for all time, and, to prove $\mathcal{U}_t^* S \mathcal{U}_t = \mathcal{S}$, one observes that

$$i\partial_t (\mathcal{U}_t^* S \mathcal{U}_t) = -(\mathcal{U}_t^* S \mathcal{U}_t) \Lambda_t S + S \Lambda_t (\mathcal{U}_t^* S \mathcal{U}_t),$$

which is a linear time-dependent ordinary differential equation for $\mathcal{U}_t^* S \mathcal{U}_t$ which also admits the constant solution \mathcal{S} . By uniqueness of the solution, one gets that $\mathcal{U}_t^* S \mathcal{U}_t = \mathcal{S}$. Hence \mathcal{U}_t is a symplectomorphism for all time.

Similarly, the derivative $i\partial_t (\mathcal{U}_t \Gamma_t \mathcal{U}_t^*)$ vanishes because, using (48) and (49),

$$i\partial_t \Gamma_t = \Lambda_t S \Gamma_t - \Gamma_t S \Lambda_t.$$

Thus $\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \mathcal{U}_0 \Gamma_0 \mathcal{U}_0^* = \Gamma_0$ for all times. \square

We choose a_t and b_t in (48) and (49) such that σ_t vanishes in the limit $t \rightarrow \infty$. Let $\mathcal{L}^1(\mathfrak{h})$ and $\mathcal{L}^2(\mathfrak{h})$ denote the spaces of trace-class and Hilbert - Schmidt operators on the space \mathfrak{h} .

Lemma 3.11. *The ordinary differential equation*

$$\partial_t \gamma_t = -2\sigma_t \bar{\sigma}_t, \quad (51)$$

$$\partial_t \sigma_t = -(\sigma_t + \sigma_t \bar{\gamma}_t + \gamma_t \sigma_t), \quad (52)$$

with initial data $\sigma_0 = \sigma$, $\gamma_0 = \gamma$ given in Prop. 3.9(i), has a unique global solution $(\gamma_t, \sigma_t) \in C^1([0, \infty); \mathcal{L}^1(\mathfrak{h}) \times \mathcal{L}^2(\mathfrak{h}))$.

Let $\Lambda_t = \begin{pmatrix} 0 & i\sigma_t \\ -i\bar{\sigma}_t & 0 \end{pmatrix}$, and $\mathcal{U}_t = \begin{pmatrix} u_t & v_t \\ \bar{v}_t & \bar{u}_t \end{pmatrix}$ and $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1+\bar{\gamma}_t \end{pmatrix}$ as in Lemma 3.10:

- \mathcal{U}_t converges in $\mathcal{H}^{\infty,2}$ to a symplectomorphism \mathcal{U}_∞ .
- $\Gamma_0 = \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* = \mathcal{U}_\infty \begin{pmatrix} \gamma_\infty & 0 \\ 0 & 1+\bar{\gamma}_\infty \end{pmatrix} \mathcal{U}_\infty^*$ with $0 \leq \gamma_\infty \leq \gamma_0$.

Proof. The existence of maximal solutions to (51) - (52) follows from the Picard-Lindelöf theorem. Now using the \mathcal{U}_t constructed in Lemma (3.10), one gets that $(\mathcal{U}_t)^{-1} \Gamma_0 (\mathcal{U}_t^*)^{-1} = \Gamma_t$, which implies that $\Gamma_t \geq 0$ and thus $\gamma_t \geq 0$. It then follows from (51) that γ_t is decreasing in the sense of quadratic forms and $\|\gamma_t\|_{\mathcal{H}^1} \leq \|\gamma_0\|_{\mathcal{H}^1}$. Using (52) and $\gamma_t \geq 0$ yields

$$\begin{aligned} \partial_t \|\sigma_t\|_{H_s^1}^2 &= \text{Tr}[-(\sigma_t + \sigma_t \bar{\gamma}_t + \gamma_t \sigma_t) \sigma_t^* M^2 - \sigma_t (\sigma_t^* + \sigma_t^* \bar{\gamma}_t + \gamma_t \sigma_t^*) M^2] \\ &\leq -2 \text{Tr}[\sigma_t \sigma_t^* M^2] = -2 \|\sigma_t\|_{H_s^1}^2. \end{aligned}$$

Hence, the estimate $\|\sigma_t\|_{H_s^1} \leq \|\sigma_0\|_{H_s^1} \exp(-t)$ follows. The pair (γ_t, σ_t) is thus bounded in $\mathcal{H}^1 \times H_s^1$ and the maximal time of the solution is $T = \infty$. We also get that $\gamma_t \rightarrow \gamma_\infty$ in \mathcal{H}^1 as $t \rightarrow \infty$ as γ_t is decreasing and bounded by below, and $\sigma_t \rightarrow 0$.

Integrating the derivative of \mathcal{U}_t^* and taking the norm of both sides yields

$$\|\mathcal{U}_t^*\|_{\mathcal{H}^{\infty,2}} \leq \|\mathcal{U}_0^*\|_{\mathcal{H}^{\infty,2}} + \int_0^t \|\sigma_s\|_{H_s^1} \|\mathcal{U}_s^*\|_{\mathcal{H}^{\infty,2}} ds. \quad (53)$$

The Grönwall lemma, combined with $\|\mathcal{U}_0^*\|_{\mathcal{H}^{\infty,2}} = 1$ and the estimate on $\|\sigma_t\|_{H_s^1}$ provide

$$\|\mathcal{U}_t^*\|_{\mathcal{H}^{\infty,2}} \leq \exp\left(\int_0^t \|\sigma_s\|_{H_s^1} ds\right) \leq \exp(\|\sigma_0\|_{H_s^1}).$$

Thus, the integral $\int_0^\infty \mathcal{S} \Lambda_s \mathcal{U}_s^* ds$ is absolutely convergent and

$$\mathcal{U}_t^* \xrightarrow[t \rightarrow \infty]{} \mathcal{U}_0^* - i \int_0^\infty \mathcal{S} \Lambda_s \mathcal{U}_s^* ds =: \mathcal{U}_\infty^*$$

in $\mathcal{H}^{\infty,2}$, and the limit \mathcal{U}_∞^* is still an implementable symplectomorphism.

Hence,

$$\Gamma_0 - \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* = \mathcal{U}_t \Gamma_t \mathcal{U}_t^* - \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* \rightarrow 0$$

as $t \rightarrow \infty$, where $\Gamma_\infty = \begin{pmatrix} \gamma_\infty & 0 \\ 0 & 1+\bar{\gamma}_\infty \end{pmatrix}$, and the convergence takes place in the space of block operators with diagonal elements in \mathcal{H}^1 and off-diagonal elements in H_s^1 . This proves the last point. \square

This completes the proof of existence. \square

Proof of uniqueness in Prop. 3.8. Indeed, let us consider γ' and γ'' satisfying the conditions of Prop. 3.8. Then there exists a symplectomorphism \mathcal{U} such that

$\begin{pmatrix} \gamma'' & 0 \\ 0 & \overline{\gamma''+1} \end{pmatrix} = \mathcal{U}^* \begin{pmatrix} \gamma' & 0 \\ 0 & \overline{\gamma'+1} \end{pmatrix} \mathcal{U}$. As $\mathcal{U}^* \mathcal{S} \mathcal{U} = \mathcal{S}$, this is equivalent to

$$\begin{pmatrix} \gamma'' + 1/2 & 0 \\ 0 & \overline{\gamma'' + 1/2} \end{pmatrix} = \mathcal{U}^* \begin{pmatrix} \gamma' + 1/2 & 0 \\ 0 & \overline{\gamma' + 1/2} \end{pmatrix} \mathcal{U} \quad (54)$$

and we want to prove that γ' and γ'' are unitarily equivalent in L^2 . The off-diagonal entries in (54) yield $u^*(\gamma' + 1/2)v + v^T(\gamma' + 1/2)\bar{u} = 0$ and as \mathcal{U} is a symplectomorphism, we get from (43) that u is invertible and $v\bar{u}^{-1} = u^{*-1}v^T$. Thus,

$$(\gamma' + \frac{1}{2})v\bar{u}^{-1} + v\bar{u}^{-1}(\gamma' + \frac{1}{2}) = 0.$$

We can now use a known method to solve the Lyapunov (or Sylvester) equations:

$$\begin{aligned} v\bar{u}^{-1} &= - \int_0^\infty \frac{d}{dt} \left(e^{-t(\gamma' + \frac{1}{2})} v\bar{u}^{-1} e^{-t(\gamma' + \frac{1}{2})} \right) dt \\ &= \int_0^\infty e^{-t(\gamma' + \frac{1}{2})} \left((\gamma' + \frac{1}{2})v\bar{u}^{-1} + v\bar{u}^{-1}(\gamma' + \frac{1}{2}) \right) e^{-t(\gamma' + \frac{1}{2})} dt = 0, \end{aligned}$$

where we used that $\gamma + 1/2 \geq 1/2$, so that there is no problem in handling the integrals. Hence $v = 0$, and, using (43) again, u is a unitary operator. And thus $\gamma'' = u^*\gamma'u$ which proves the result. \square

We now write the HFB equations in a form that is reminiscent of a Hamiltonian structure, and use it to give a direct proof of the conservation of the energy.

Notation: For $\phi \in H^1$, $\mathcal{U} = \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \in \mathcal{H}^{\infty,2}$ a symplectomorphism, and $\gamma'_0 \in \mathcal{H}^1$ non-negative. We set

$$\begin{aligned} \mathcal{H}_{\gamma'_0}(\phi, u, v) &:= \langle \phi, h\phi \rangle + \text{Tr}[(u^*\gamma'_0 u + v^T(1 + \bar{\gamma}'_0)\bar{v})(h + b[|\phi\rangle\langle\phi|])] \\ &\quad + \frac{1}{2} \text{Tr}[(u^*\gamma'_0 u + v^T(1 + \bar{\gamma}'_0)\bar{v})b[u^*\gamma'_0 u + v^T(1 + \bar{\gamma}'_0)\bar{v}]] \\ &\quad + \frac{1}{2} \text{Tr}[k[u^*\gamma'_0 v + v^T(1 + \bar{\gamma}'_0)\bar{u} + |\phi\rangle\langle\bar{\phi}|](v^*\gamma'_0 u + u^T(1 + \bar{\gamma}'_0)\bar{v} + |\bar{\phi}\rangle\langle\phi|)]. \end{aligned}$$

In the next proposition and its proof we use the abbreviations $h(t) \equiv h(\gamma_t^{\phi_t})$ and $k(t) \equiv k(\sigma_t^{\phi_t})$, where, recall, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + \phi \otimes \phi$, and $h(\gamma)$ and $k(\sigma)$ are defined in (29) and (30).

Proposition 3.12. *Let $\rho_t = (\phi_t, \gamma_t, \sigma_t) \in C^0([0, T]; X^3) \cap C^1([0, T]; X^1)$ be a solution to the HFB equations (26)~(28) in the classical sense, on an interval $[0, T]$, with $T > 0$. Let \mathcal{U}_t and γ'_0 be as in Proposition 3.9.*

Then $\mathcal{E}(\phi_t, \gamma_t, \sigma_t) = \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t)$ and the derivatives of $\mathcal{H}_{\gamma'_0}$ and of (ϕ_t, u_t, v_t) are linked through the equations

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \langle \phi |}(\phi_t, u_t, v_t) = i\partial_t \phi_t, \quad (55)$$

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t) = \gamma'_0 i\partial_t u_t + \frac{1}{2} v_t \overline{k(t)}, \quad (56)$$

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t) = -\gamma'_0 i\partial_t v_t + v_t \overline{h(t)} + \frac{1}{2} u_t k(t). \quad (57)$$

The conservation of the energy $\mathcal{E}(\phi_t, \gamma_t, \sigma_t)$ follows.

Proof. Eq. (46) is equivalent to

$$\begin{aligned}\gamma_t &= u_t^* \gamma'_0 u_t + v_t^T (1 + \bar{\gamma}'_0) \bar{v}_t, \\ \sigma_t &= u_t^* \gamma'_0 v_t + v_t^T (1 + \bar{\gamma}'_0) \bar{u}_t.\end{aligned}$$

Hence, we can rewrite the expression of the energy in terms of ϕ_t , u_t , and v_t as $\mathcal{E}(\phi_t, \gamma_t, \sigma_t) = \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t)$. We then compute the derivatives of $\mathcal{H}_{\gamma'_0}$:

$$\begin{aligned}\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \langle \phi |}(\phi, u, v) &= h\phi + b[u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}] \phi + k[\sigma + \phi \otimes \phi] |\bar{\phi}\rangle, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi, u, v) &= \gamma'_0 u (h + b[|\phi\rangle \langle \phi|] + b[u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}]) \\ &\quad + \left(\frac{1}{2} + \gamma'_0\right) v k[v^* \gamma'_0 u + u^T (1 + \bar{\gamma}'_0) \bar{v} + |\bar{\phi}\rangle \langle \phi|], \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi, u, v) &= (1 + \gamma'_0) v (\bar{h} + b[|\bar{\phi}\rangle \langle \bar{\phi}|] + b[u^T \bar{\gamma}'_0 \bar{u} + v^* (1 + \gamma'_0) v]) \\ &\quad + \left(\frac{1}{2} + \gamma'_0\right) u k[u^* \gamma'_0 v + v^T (1 + \bar{\gamma}'_0) \bar{u} + |\phi\rangle \langle \bar{\phi}|].\end{aligned}$$

Replacing (ϕ, u, v) by (ϕ_t, u_t, v_t) yields

$$\begin{aligned}\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \langle \phi |}(\phi_t, u_t, v_t) &= h\phi_t + b[\gamma_t] \phi_t + k(t) \bar{\phi}_t, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t) &= \gamma'_0 u_t h(t) + \left(\frac{1}{2} + \gamma'_0\right) v_t \overline{k(t)}, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t) &= (1 + \gamma'_0) v_t \overline{h(t)} + \left(\frac{1}{2} + \gamma'_0\right) u_t k(t),\end{aligned}$$

which are in fact (55), (56), (57) using the HFB equations. Hence, using first the chain rule, then (55), (56), and (57),

$$\begin{aligned}\frac{d}{dt} \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t) &= \langle \partial_t \phi_t | \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \langle \phi |}(\phi_t, u_t, v_t) + \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial |\phi\rangle}(\phi_t, u_t, v_t) | \partial_t \phi_t \rangle \\ &\quad + \text{Tr}[\partial_t u_t^* \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t)] + \text{Tr}[\partial_t u_t \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u}(\phi_t, u_t, v_t)] \\ &\quad + \text{Tr}[\partial_t v_t^* \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t)] + \text{Tr}[\partial_t v_t \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v}(\phi_t, u_t, v_t)] \\ &= \Re \text{Tr}[\partial_t u_t^* v_t \overline{k(t)} + \partial_t v_t^* (v_t \overline{h(t)} + \frac{1}{2} u_t k(t))].\end{aligned}$$

We can now use that the evolution equation (45) on \mathcal{U}_t is equivalent to

$$i\partial_t u_t = u_t h(t) + v_t \overline{k(t)}, \quad (58)$$

$$i\partial_t v_t = -u_t k(t) - v_t \overline{h(t)}, \quad (59)$$

along with $\text{Tr}[A^T] = \text{Tr}[A]$ and the cyclicity of trace to group all the terms as in

$$\begin{aligned}\frac{d}{dt} \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t) &= \Im \text{Tr}[\overline{k(t)} h(t) (v_t^T \bar{u}_t - u_t^* v_t) - \overline{k(t)} k(t) v_t^* v_t \\ &\quad + \overline{k(t)} h(t) v_t^T \bar{u}_t + 2h(t) h(t) v_t^T \bar{v}_t + \overline{k(t)} k(t) u_t^T \bar{u}_t + h(t) k(t) u_t^T \bar{v}_t]\end{aligned}$$

this article	$\phi(x)$	$\gamma(x; x)$	$\sigma(x, x)$	$h_{g\delta}$	$k_{g\delta}$	N_j	V
[15]	$\Phi(\mathbf{r})$	$\tilde{n}(\mathbf{r})$	$\tilde{m}(\mathbf{r})$	\mathcal{L}	$gm(\mathbf{r})$	$N_0(E_j)$	$U_{ext} - \mu$

TABLE 1. Correspondence between the notations of this article and some notations common in the physics literature [15].

which then vanishes since $v_t^T \bar{u}_t = u_t^* v_t$ for a symplectomorphism (see (43)), and the terms $\overline{k(t)}k(t)v_t^* v_t$, $h(t)h(t)v_t^T \bar{v}_t$, $\overline{k(t)}k(t)u_t^T \bar{u}_t$, and $\overline{k(t)}h(t)v_t^T \bar{u}_t + h(t)k(t)u_t^T \bar{v}_t$ give real traces. \square

4. RELATION WITH THE HFB EIGENVALUE EQUATIONS

In this section, we link our work with the HFB eigenvalue equations often encountered in the physics literature [15, 14, 32].

To be explicit, we give, in Table 1, the correspondence between the notations of this article and those of an article of Griffin [15]. We note that the setting in [15] is not exactly the same as ours, since the class of external potentials V that we consider excludes trapping potentials, and the solutions $\Phi(\mathbf{r})$ considered in [15] are time-independent. Moreover, we note that in this paper, we give rigorous proofs in the case of a two-body interaction potential v such that v^2 is relatively form-bounded with respect to the Laplacian, which excludes potentials as singular as $g\delta$; hence, the correspondence we establish in this section is only formal. Nevertheless, we believe that pointing out this relationship is useful.

Moreover, we note that in the physics literature (see e.g., [15, (23)]), the HFB eigenvalue equations are often investigated using a generalized eigenbasis decomposition (using vectors often denoted by u_j , v_j which play the same role as below), which we can relate to our approach in the following manner, based on our discussion from Section 3.

Let $\mathcal{U}_t = \begin{pmatrix} u_t & v_t \\ \bar{u}_t & \bar{v}_t \end{pmatrix}$, and let $\gamma'_0 \geq 0$ be a trace class operator as in Prop. 3.9, with the orthonormal decomposition $\gamma'_0 = \sum_{j \geq 0} N_j |\zeta_j\rangle \langle \zeta_j|$. Let

$$u_{j,t} := u_t^* \zeta_j \quad \text{and} \quad v_{j,t} := -v_t^* \zeta_j.$$

Then (46) yields

$$\begin{aligned} \gamma_t &= \sum_{j \geq 0} (N_j |u_{j,t}\rangle \langle u_{j,t}| + (1 + N_j) |\bar{v}_{j,t}\rangle \langle \bar{v}_{j,t}|), \\ \sigma_t &= \sum_{j \geq 0} (N_j |u_{j,t}\rangle \langle v_{j,t}| + (1 + N_j) |\bar{v}_{j,t}\rangle \langle \bar{u}_{j,t}|). \end{aligned}$$

which yield [15, (25)] by evaluation on the diagonal:

$$\gamma_t(x; x) = \sum_{j \geq 0} (N_j |u_{j,t}(x)|^2 + (1 + N_j) |\bar{v}_{j,t}(x)|^2), \quad (60)$$

$$\sigma_t(x, x) = \sum_{j \geq 0} u_{j,t}(x) \bar{v}_{j,t}(x) (1 + 2N_j). \quad (61)$$

We now consider a pair interaction potential $v = g\delta$. We assume that ϕ is independent of time and $u_{j,t}, v_{j,t}$ have the simple form

$$u_{j,t} = e^{-itE_j} u_{j,0}, \quad v_{j,t} = e^{-itE_j} v_{j,0}. \quad (62)$$

We also distinguish the quantities corresponding to $v = g\delta$ by the index $g\delta$. Then (45) formally yields the HFB eigenvalue equations

$$\begin{aligned} h_{g\delta} u_j - k_{g\delta} v_j &= E_j u_j, \\ \overline{h_{g\delta}} v_j - \overline{k_{g\delta}} u_j &= -E_j v_j, \end{aligned}$$

as presented in the work of Griffin [15, (23)]. Note that (60), (61), and (62) imply that $\gamma_t(x; x)$ and $\sigma_t(x; x)$ are time independent, since the phases simplify.

We conclude that the HFB eigenvalue equations are the stationary version of our equation (45). It amounts to finding eigenvalues and eigenvectors for the matrix $\Lambda\mathcal{S}$ in (45), which is a nonlinear problem since Λ depends on γ and σ (that is, on u, v and γ'_0). Furthermore, the decomposition in functions u_j and v_j corresponds to a “diagonalization” of the generalized one-particle density matrix Γ in the sense of Proposition 3.8.

5. EXISTENCE AND UNIQUENESS OF SOLUTIONS TO THE HFB EQUATIONS

We prove the global in time existence and uniqueness of mild solutions to the time-dependent Hartree-Fock-Bogoliubov equations in the H^1 -setting, and for a class of interaction potentials including the Coulomb potential. The proof is based on a standard fixed point argument (through an application of the Cauchy-Lipschitz and Picard-Lindelöf theorem in the proof of Theorem 5.1).

Let X be a Banach space, $f \in C(X)$ a continuous function on X , and $-iA$ the infinitesimal generator of a strongly continuous semigroup $G(t)$ such that $\|G(t)\| \leq \exp(\kappa t)$, for all $t \geq 0$ with a fixed $\kappa \in \mathbb{R}$. We say that a continuous function $\rho : [0, T] \rightarrow X$ is a *mild solution* of the problem

$$\begin{cases} i\partial_t \rho &= A\rho + f(\rho), \\ \rho(0) &= \rho_0 \in X, \end{cases} \quad (63)$$

if ρ_t solves the fixed point equation in integral form

$$\rho_t = G(t)\rho_0 - i \int_0^t G(t-s)f(\rho_s) ds \quad (64)$$

(with the integral in Bochner’s sense).

In what follows we will use the space $X = X^1$. Moreover, A determines the linear part in the HFB equations and f the nonlinear part. (The explicit form of A and f is given in Eq. (66) and Eq. (67).)

Theorem 5.1. *Let $d \leq 3$ and $\rho_0 = (\phi_0, \gamma_0, \sigma_0) \in X^1$. Assume that the potentials V and v are such that*

- V is infinitesimally form-bounded with respect to the Laplacian,
- v is symmetric, $v(x) = v(-x)$, and such that $v^2 \leq CM^2$ for some $C > 0$.

Then the following hold:

- (1) *Existence and uniqueness of a local mild solution:*

There exists a unique maximal solution

$$(\rho_t)_{t \in [0, T)} = (\phi_t, \gamma_t, \sigma_t)_{t \in [0, T)} \in C^0([0, T); X^1)$$

to the HBF equations (26) to (28) in the mild sense, for some $0 < T \leq \infty$.

- (2) *Existence and uniqueness of a local classical solution:*

If $\rho_0 \in X^3$, then

$$(\rho_t)_{t \in [0, T)} \in C^0([0, T); X^3) \cap C^1([0, T); X^1)$$

and ρ_t satisfies the HBF equations (26) to (28) in the classical sense.

- (3) *Conservation laws:*

The number of particles $\text{Tr}[\gamma_t]$ and the energy (35) are constants.

- (4) *Existence of a global solution:*

If additionally $\Gamma_0 \geq 0$, then the solution is global, i.e., $T = \infty$.

Remark 5.2. The class of potentials v considered here includes the repulsive Coulomb potential, as can be seen using the Hardy-Rellich inequality.

Proof of Theorem 5.1.(1) [Local Mild Solutions]. We use the notations introduced at the beginning of Section 2. Separating the linear part $A\rho$ and nonlinear part $f(\rho)$, we can write the HFB equations (26) to (28) in the form

$$i\partial_t \rho = A\rho + f(\rho), \quad (65)$$

where $\rho := (\phi, \gamma, \sigma) \in X^2$. Then the linear part in the HFB equations is given by

$$A\rho = (h\phi, [h, \gamma], [h, \sigma]_+ + k[\sigma]), \quad (66)$$

and the nonlinear part $f := (f_1, f_2, f_3)$ by

$$f_1(\rho) = b[\gamma]\phi + k[\sigma + \phi^{\otimes 2}]\bar{\phi}, \quad (67)$$

$$f_2(\rho) = [b[\gamma + |\phi\rangle\langle\phi|], \gamma] + k[\sigma + \phi^{\otimes 2}]\bar{\sigma} - \sigma \overline{k[\sigma + \phi^{\otimes 2}]}, \quad (68)$$

$$f_3(\rho) = [b[\gamma + |\phi\rangle\langle\phi|], \sigma]_+ + [k[\sigma + \phi^{\otimes 2}], \gamma]_+. \quad (69)$$

From Lemma 5.4, below, we obtain that f is continuously Fréchet differentiable in X^1 and therefore is locally Lipschitz, and from Lemma 5.3, we obtain that $G(t) = \exp(itA)$ defines a strongly continuous uniformly bounded semigroup on X^1 .

Consequently, we can rewrite the HFB equations (26) - (28) as a fixed point problem

$$\rho_t = G(t)\rho_0 - i \int_0^t G(t-s)f(\rho_s) ds.$$

and use the Banach contraction theorem to show that (26) - (28) have the unique local mild solution in X^1 for the given initial data. (For the details for this standard argument, see [24], Section 9.2e, Theorem 3.) \square

We will now prove our main Lemmata on $G(t) = \exp(itA)$ and f . First, we introduce norms used below:

$$\|\phi\|_{H^j} := \|M^j \phi\|_{L^2(\mathbb{R}^d)}, \quad \|\gamma\|_{\mathcal{H}^j} := \|M^j \gamma M^j\|_{\mathcal{L}^1},$$

$$\|\sigma\|_{H_s^j} := \|(M^2 \otimes 1 + 1 \otimes M^2)^{j/2} \sigma\|_{L^2(\mathbb{R}^{2d})}.$$

Lemma 5.3. *If V is infinitesimally form-bounded with respect to the Laplacian, and v is symmetric, $v(x) = v(-x)$, and such that $v^2 \leq CM^2$ for some $C > 0$, then $G(t) = \exp(itA)$ defines a strongly continuous, uniformly bounded semigroup on X^1 , i.e., the map $t \mapsto \|G(t)\|_{\mathcal{B}(X^1)}$ is bounded.*

Note that the proof Lemma 5.3 uses that $-\Delta$ is h -bounded, and h is $-\Delta$ -bounded. The latter condition does not hold for confining potentials. The proof also uses the translation invariance of M .

Proof. The letter C denotes a constant, which changes along the computations below. For $(\phi, \gamma, \sigma) \in X^1$,

$$\begin{aligned} \|\exp(-ith)\phi\|_{H^1}^2 &= \langle \phi, \exp(ith)M^2 \exp(-ith)\phi \rangle \\ &\leq \langle \phi, \exp(ith)(h+k) \exp(-ith)\phi \rangle = \langle \phi, (h+k)\phi \rangle \leq C\|\phi\|_{H^1}^2 \end{aligned}$$

for some $k > 0$. Similarly $\|\exp(-ith)\gamma \exp(ith)\|_{\mathcal{H}^1} \leq C\|\gamma\|_{\mathcal{H}^1}$. Finally, with $\tilde{h} = h \otimes 1 + 1 \otimes h + v(x-y)$, as quadratic forms on $L^2(\mathbb{R}^{2d})$, using that $v \leq CM \leq CM^2$,

$$\begin{aligned} \exp(i\tilde{h})(M^2 \otimes 1 + 1 \otimes M^2) \exp(-i\tilde{h}) \\ \leq \exp(i\tilde{h})(\tilde{h} + 2k) \exp(-i\tilde{h}) = \tilde{h} + 2k \leq 2C(M^2 \otimes 1 + 1 \otimes M^2) \end{aligned}$$

and thus $\|\exp(-i\tilde{h})\sigma\|_{H_s^1} \leq C\|\sigma\|_{H_s^1}$ which completes the proof. \square

The estimates on the operators b and k of Lemma E.1 allow us to control the nonlinear term f in the HFB equations.

Lemma 5.4. *Assume that the pair interaction potential v is symmetric, $v(x) = v(-x)$, and that $v^2 \leq CM^2$ for some $C > 0$.*

Then the vector of nonlinear terms $f = (f_1, f_2, f_3)$ defined in Eq. (67)–(69) is continuously Fréchet differentiable in X^1 ($f \in C^1(X^1)$).

Proof of Lemma 5.4. Each f_j is a linear combination of multi-linear maps. It is thus enough to prove continuity estimates for each of those multi-linear terms to prove that f is both well defined and Fréchet differentiable. It is sufficient to prove that, for the quadratic part

$$\begin{aligned} \|(b[\gamma]\phi + k[\sigma]\bar{\phi}, [b[\gamma], \gamma] + k[\sigma]\bar{\sigma} - \sigma\overline{k[\sigma]})\|_{X^1} \\ \leq C\|\rho\|_{X^1}^2, \end{aligned}$$

and, for the cubic part

$$\begin{aligned} \|(k[\phi^{\otimes 2}]\bar{\phi}, [b[\phi]\langle\phi\rangle, \gamma] + k[\phi^{\otimes 2}]\bar{\sigma} - \sigma\overline{k[\phi^{\otimes 2}]})\|_{X^1} \\ \leq C\|\rho\|_{X^1}^3. \end{aligned}$$

All the cubic estimates can be deduced from their quadratic counterparts using

$$\|\phi\|\langle\phi\rangle\|_{\mathcal{H}^1} \leq \|\phi\|_{H^1}^2 \quad \text{and} \quad \|\phi \otimes \phi\|_{H_s^1} \leq \|\phi\|_{H^1}^2.$$

We thus only consider the quadratic terms. We estimate $[b[\gamma], \gamma]$ using Lemma. E.1.(1)

$$\begin{aligned} \| [b[\gamma], \gamma] \|_{\mathcal{H}^1} &\leq 2 \| Mb[\gamma] M^{-1} M \gamma M \|_{\mathcal{L}^1(L^2(\mathbb{R}^d))} \\ &\leq 2 \| b[\gamma] \|_{\mathcal{H}^1} \| \gamma \|_{\mathcal{H}^1} \leq C \| \gamma \|_{\mathcal{H}^1}^2 \leq C \| \rho \|_{X^1}^2. \end{aligned}$$

The term $[b[\phi]\langle\phi\rangle, \gamma]$ is controlled with the same method. Let us give the estimates for the first term $b[\gamma]\phi$ in full detail. Using Lemma E.1.(1)

$$\| (b[\gamma]\phi, 0, 0) \|_{X^1} = \| b[\gamma]\phi \|_{H^1} \leq C \| \gamma \|_{\mathcal{H}^1} \| \phi \|_{H^1} \leq C \| \rho \|_{X^1}^2.$$

For the other terms we only give the main steps, using Lemma. E.1 each time. For $k[\sigma]\bar{\phi}$, using Lemma E.1.(2),

$$\| K[\sigma]\bar{\phi} \|_{H^1} \leq \| Mk[\sigma] M^{-1} \|_{\mathcal{B}(L^2(\mathbb{R}^d))} \| M\bar{\phi} \|_{L^2} \leq C \| \sigma \|_{H_s^1} \| \phi \|_{H^1}.$$

For $k[\sigma]\bar{\sigma}$ (or similarly $\sigma\overline{k[\sigma]}$), using Lemma E.1.(2),

$$\begin{aligned} \| k[\sigma]\bar{\sigma} \|_{\mathcal{H}^1} &= \| Mk[\sigma] M^{-1} M\bar{\sigma} M \|_{\mathcal{L}^1(L^2(\mathbb{R}^d))} \\ &\leq \| Mk[\sigma] M^{-1} \|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} \| M\bar{\sigma} M \|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} \leq C \| \sigma \|_{H_s^1}^2. \end{aligned}$$

For $b[\gamma]\sigma$ (or similarly $\sigma\overline{b[\gamma]}$), using Lemma E.1.(1),

$$\| b[\gamma]\sigma \|_{H_s^1} \leq \| Mb[\gamma] M^{-1} \|_{\mathcal{B}(L^2(\mathbb{R}^d))} \| M\sigma M \|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} \leq C \| \gamma \|_{\mathcal{H}^1} \| \sigma \|_{H_s^1}.$$

And finally $k[\sigma]\bar{\gamma}$ (or similarly $\gamma\overline{k[\sigma]}$), using Lemma E.1.(2),

$$\| k[\sigma]\bar{\gamma} \|_{H_s^1} \leq \| Mk[\sigma] M^{-1} \|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} \| M\bar{\gamma} M \|_{\mathcal{B}(L^2(\mathbb{R}^d))} \leq C \| \sigma \|_{H_s^1} \| \gamma \|_{\mathcal{H}^1},$$

which completes the proof. \square

Proof of Theorem 5.1.(2) [Local Classical Solutions]. The existence of classical solutions to the HFB equations for initial data in X^3 then follows from:

Lemma 5.5 (See [35, Lemma 3.1]). *If $-iA$ is the generator of a continuous one-parameter semi-group in the Banach space X , and if f is continuously differentiable on X , then a mild solution of Eq. (63) has its values in the domain $\mathcal{D}(A)$ of A throughout its interval of existence provided this is the case initially.*

In other words, ρ_t , if it exists at all, then satisfies the differential equation (63) in the obvious sense. \square

Proof of Theorem 5.1.(3) [Conservation Laws]. For classical solutions, the conservation of the number particle and of the energy were proven as consequences of the same conservation laws for the many body system in Theorem 2.8 and 2.5. Another proof of the conservation law for the energy using only the HFB equations (independently from the many body problem) was given in Prop. 3.12, and the conservation of the particle number could also be proven directly from (27). We can now use those results since we proved the local existence of a classical solution. The conservation laws then extend to mild solutions by approximation. \square

Proof of Theorem 5.1.(4) [Global Solution]. We recall that for a maximal solution ρ_t of the mild problem (64) defined on an interval $[0, T)$, we have that either $T = \infty$

or $\sup_{t \in [0, T)} \|\rho_t\|_{X^1} = \infty$ (see, e.g., Theorem 4.3.4 in [10]). It is thus enough to prove that

$$\sup_{t \in [0, T)} \{ \|\phi_t\|_{H^1}, \|\gamma_t\|_{\mathcal{H}^1}, \|\sigma_t\|_{H_s^1} \} < \infty$$

to show that the solutions are global.

Let

$$\mathbb{T} := \int dx dy \psi^*(x) (-\Delta) \psi(y), \quad (70)$$

Because V is infinitesimally form bounded with respect to the Laplacian,

$$\int dx \psi^*(x) \psi(x) V(x) \geq -\frac{1}{3} \mathbb{T} - c\mathbb{N} \quad (71)$$

holds. And, because $v^2 \leq CM^2$, it follows that, for any $\varepsilon \in (0, 1]$,

$$|v| \leq \sqrt{C(1 - \Delta)} \leq \varepsilon(1 - \Delta) + C\varepsilon^{-1} \leq -\varepsilon\Delta + C\varepsilon^{-1}. \quad (72)$$

(We write C for constants which depend on v , d and change along the estimates.) Applying this with $\varepsilon = 1/(3(n-1))$,

$$v(x-y) \geq -\frac{1}{6(n-1)} (-\Delta_x - \Delta_y) - C(n-1). \quad (73)$$

Then, summing the $n(n-1)/2$ terms of this form on each n -particles subspace of the Fock space, we obtain that

$$\mathbb{V} := \frac{1}{2} \int dx dy v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) \geq -\frac{1}{3} \mathbb{T} - C\mathbb{N}^3. \quad (74)$$

Hence, from the definition of \mathbb{H} , (71) and (74) we get

$$\mathbb{T} \leq 3\mathbb{H} + C\mathbb{N}^3. \quad (75)$$

We now take the expectation value of ω_t^q . Using the conservation of the particle number and of the energy,

$$\mathrm{Tr}[-\Delta(\gamma_t + |\phi_t\rangle\langle\phi_t|)] \leq C(\mathcal{E}(\phi_t, \gamma_t, \sigma_t) + \mathcal{N}(\phi_t, \gamma_t, \sigma_t)^3 + 1) \quad (76)$$

$$\leq C(\mathcal{E}(\phi_0, \gamma_0, \sigma_0) + \mathcal{N}(\phi_0, \gamma_0, \sigma_0)^3 + 1). \quad (77)$$

Combined with the conservation of the particle number, this estimate provides bounds on $\|\gamma_t\|_{\mathcal{H}^1}$ and $\|\phi_t\|_{H^1}$ that are uniform in t . Moreover, uniform bounds on $\|\sigma_t\|_{H_s^1}$ are then obtained from Proposition 3.1. It thus follows that the solution is global, as claimed. \square

6. GIBBS STATES AND BOSE-EINSTEIN CONDENSATION

In this section, we determine translation- and $U(1)$ gauge-invariant Gibbs states for the HFB equations without an external potential, and with an interaction potential $g\delta$, and discuss the emergence of a Bose-Einstein condensate at positive temperature. (Recall from the introduction that $U(1)$ gauge-invariant Gibbs states for the HFB equations are, in fact, Gibbs states for the Hartree-Fock equations.)

We consider the system on a torus, $\Lambda_L = \mathbb{R}^d/2L\mathbb{Z}^d$, i.e., $[-L, L]^d$ with periodic boundary conditions. Accordingly, we denote $\Lambda_L^* := \frac{\pi}{L}\mathbb{Z}^d$ the lattice reciprocal to

$2L\mathbb{Z}^d$. We will eventually take the thermodynamic limit, $L \rightarrow \infty$, and discuss the emergence of a Bose-Einstein condensate.

The Hamiltonian \mathbb{H} of the Bose gas is $U(1)$ gauge-invariant (that is, invariant under the transformation $\psi^\sharp \rightarrow (e^{i\theta}\psi)^\sharp$), and, as we consider the case with no external potential, translation invariant. On a compact torus, where the volume is finite, these symmetries are also present in the Gibbs states of system (the notion of translation invariance should be, of course, appropriately modified). We are interested in quasifree states ω_L^q which on the one hand satisfy both the $U(1)$ gauge invariance and the translation invariance, and, on the other hand satisfy a fixed point equation corresponding to the consistency condition (32) in the dynamical case:

$$\Phi(\omega_L^q) = \omega_L^q \quad \text{with} \quad \Phi(\omega_L^q)(\mathbb{A}) := \text{Tr}[\mathbb{A} \exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q) - \mu\mathbb{N}))]/\Xi \quad (78)$$

where $\beta > 0$ is the inverse temperature, μ is the chemical potential, and $\Xi = \text{Tr}[\exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q) - \mu\mathbb{N}))]$. The $U(1)$ gauge-invariance of ω_L^q then implies that the truncated expectations $\phi_{\omega_L^q}$ and $\sigma_{\omega_L^q}$ vanish. Indeed, if one of them was non-zero, then the HFB Hamiltonian \mathbb{H}_{HFB} would include terms which would break $U(1)$ gauge invariance, such as $\int dx m(x) \psi^*(x)\psi^*(x) + h.c.$. The quasifree states we consider are thus characterized by their truncated expectation γ_L , and we will replace the variable ω_L^q by γ_L in the sequel of this section.

We use the expression of the HFB Hamiltonian (31) with $v = g\delta$ (and $\phi = 0, \sigma = 0$), although this expression was derived for more regular interaction potentials v 's:

$$\mathbb{H}_{HFB}(\omega_L^q) = \int dx dy \psi^*(x)\psi(y) (-\Delta + gn)(x; y), \quad (79)$$

with $n = n(x) = \gamma_L(x; x)$. The translation invariance implies that the kernel $\gamma_L(x; y)$ is a function of $x - y$, that we still denote by γ_L , and therefore $n = n(x) = \gamma_L(x; x)$ is independent of x .

Applying the fixed point equation (78) with $\mathbb{A} = \psi^*(y)\psi(x)$ one can express it equivalently in the variable γ_L :

$$\gamma_L = \frac{1}{\exp(\beta(-\Delta + gn\mathbf{1} - \mu\mathbf{1})) - \mathbf{1}}, \quad (80)$$

for $n \in [0, \infty)$. The operator γ_L is a pseudodifferential operator with symbol

$$\hat{\gamma}_L(k) := \int_{\Lambda_L} \gamma_L(x) e^{-ix \cdot k} dx = \frac{1}{\exp(\beta(k^2 + gn - \mu)) - \mathbf{1}} \quad (81)$$

of γ_L . Thus

$$n = \gamma_L(0) = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k). \quad (82)$$

As the Fourier coefficients of γ_L depend only of the number n , we obtain from (80), (81) and (82) a *nonlinear fixed point equation* for n :

$$n = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1}. \quad (83)$$

Note that the knowledge of n satisfying (83), or of γ_L satisfying (80) or of ω_L^q satisfying (78) are equivalent.

From a physical point of view, it is natural to fix the density n , which can be tuned in an experiment and to compute μ . So n will be a parameter and we will solve (83) with the unknown μ .

Lemma 6.1. *Let $g, \beta, n > 0$, and, for $d \geq 3$. Let n_c be the critical density*

$$n_c := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{e^{\beta k^2} - 1} = \frac{\zeta(\frac{d}{2})\Gamma(\frac{d}{2})}{(2\pi)^d} \beta^{-\frac{d}{2}}, \quad (84)$$

where $\zeta(x) = \sum_{n \geq 1} n^{-x}$ and $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$.

We define $S_L : (-\infty, gn) \rightarrow \mathbb{R}$ and $S_\infty : (-\infty, gn] \rightarrow \mathbb{R}$ through

$$S_L(\mu) := \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1},$$

$$S_\infty(\mu) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{\exp(\beta(k^2 + gn - \mu)) - 1}.$$

Then:

- There exists a unique $\mu_L(n) < gn$ such that (83) holds, i.e.,

$$n = S_L(\mu_L(n)). \quad (85)$$

- If $n < n_c$, there exists a unique $\mu_\infty(n) < gn$ such that

$$n = S_\infty(\mu_\infty(n)). \quad (86)$$

We extend the function μ_∞ to $(0, \infty)$ by setting $\mu_\infty(n) = gn$ for $n \geq n_c$.

Remark 6.2. *The critical density n_c can be explicitly computed.*

Proof. In the discrete case, the existence follows from the intermediate value theorem because the map S_L is continuous with limits 0 at $-\infty$ and ∞ at gn . The map S_L is strictly increasing and thus there exists a unique $\mu_L(n)$ such that $n = S_L(\mu_L(n))$.

In the continuous case, we first prove the existence of $\mu_\infty(n)$, for a given $n > 0$, the map $(0, gn] \ni \mu \mapsto S_\infty(\mu)$ is well defined, continuous, $\lim_{\mu \rightarrow -\infty} S_\infty(\mu) = 0$, $S_\infty(gn) = n_c$, and thus the intermediate value theorem yields the existence of a μ_∞ satisfying (86). Since S_∞ is strictly increasing, the uniqueness follows. \square

In Theorem 6.3, we prove that the thermodynamic limit γ_∞ of the self-consistent equation (80) for γ_L is well defined and exhibits the so called Bose-Einstein condensation.

Theorem 6.3. *Let $g, \beta, n > 0$ and $d \geq 3$. Let γ_L , n_c , μ_L and μ_∞ as defined in (80) and Lemmata 6.1. Then*

$$\mu_L(n) \xrightarrow{L \rightarrow \infty} \mu_\infty(n) \quad \text{and} \quad \gamma_L \xrightarrow{L \rightarrow \infty} \gamma_\infty, \quad (87)$$

where

$$\hat{\gamma}_\infty(k) = \max\{0, n - n_c\} \delta(k) + \frac{1}{\exp(\beta(k^2 + gn - \mu_\infty(n))) - 1}. \quad (88)$$

Remark 6.4. *The presence of the $\delta(k)$ term is interpreted as the existence of Bose-Einstein condensation, because there is an accumulation of particles in the zero mode. It occurs when $\beta^{d/2}n \geq C_d$ with C_d a constant depending only on the dimension.*

Proof of Theorem 6.3. First we prove the convergence of $\mu_L(n)$ towards a $\mu_\infty(n)$. We first remark that $\mu_L(n) \geq -C$ for some constant $C > 0$ independent of L . (Otherwise one could extract a subsequence such that $n = S_{L_j}(\mu_{L_j}(n)) \rightarrow 0 < n$.) Thus the accumulation points of $\mu_L(n)$ are contained in $[-C, gn]$. Let $\mu_{L_j}(n)$ denote an extracted sequence converging to an accumulation point μ' .

In the case $n < n_c$: If $\mu' = gn$ then for j large enough $\mu_{L_j}(n) \geq (\mu_\infty(n) + gn)/2$, thus

$$n = S_{L_j}(\mu_{L_j}(n)) \geq S_{L_j}\left(\frac{gn + \mu_\infty(n)}{2}\right) \rightarrow S_\infty\left(\frac{gn + \mu_\infty(n)}{2}\right) > S_\infty(\mu_\infty(n)) = n$$

and which would lead to a contradiction. Note that it is crucial that $\mu_\infty(n) < gn$ for $n < n_c$ to get the convergence to the integral $S_\infty\left(\frac{gn + \mu_\infty(n)}{2}\right)$. It thus follows that $\mu' < gn$. Then $S_{L_j}(\mu_{L_j}(n))$ converges to n , because by definition of $\mu_L(n)$ this sum is equal to n , and also to $S_\infty(\mu')$. (One has to control the dependency in $\mu_{L_j}(n)$ in the Riemann sums.) Hence $\mu' = \mu_\infty(n)$ and the unique accumulation point is $\mu_\infty(n)$. We thus proved the convergence of $\mu_L(n)$ to $\mu_\infty(n)$.

In the case $n \geq n_c$, we sketch an argument similar to the one above. If an accumulation point μ' was such that $\mu' < gn$, then the sums $S_{L_j}(\mu_{L_j}(n))$ would converge to integrals with a value strictly smaller than n_c and thus strictly smaller than n . This would lead to a contradiction. Thus the only possible accumulation point is gn and $\mu_L(n) \rightarrow gn = \mu_\infty(n)$.

We now prove the convergence of γ_L towards γ_∞ . Let $\varphi \in C_0^\infty(\mathbb{R}^d)$. For L large enough the support of φ is included in Λ_L , and

$$\int_{\Lambda_L} \gamma_L \varphi = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k) \hat{\varphi}(k). \quad (89)$$

On the other hand $\langle \gamma_\infty, \varphi \rangle_{\mathcal{D}'} = \langle \gamma_\infty, \varphi \rangle_{S'} = \langle \hat{\gamma}_\infty, \hat{\varphi} \rangle_{S'}$ (Note that in the normalization we choose, the Fourier coefficients of φ on Λ_L and the Fourier transform coincide, there is thus no need to specify the hat notation.) The convergence of γ_L to γ_∞ is thus equivalent to

$$\frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k) \hat{\varphi}(k) \rightarrow \max\{0, n - n_c\} \hat{\varphi}(0) + \int_{\mathbb{R}^d} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta(k^2 + gn - \mu_\infty(n))} - 1}. \quad (90)$$

for all φ .

In the case $n < n_c$ the convergence is thus just a convergence of Riemann sums of the integral (with the small additional difficulty that $\mu_L(n)$ depends on L in the sum) because there is no singularity in the function $k \mapsto (\exp(\beta(k^2 + gn - \mu_\infty(n))) - 1)^{-1}$.

In the case $n \geq n_c$: Let $\varepsilon > 0$. First note that, for any fixed $\eta > 0$

$$\frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| > \eta}} \frac{\hat{\varphi}(k)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} \rightarrow \int_{|k| > \eta} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta k^2} - 1},$$

as $L \rightarrow \infty$. We choose $\eta > 0$ small enough so that

$$|k| \leq \eta \Rightarrow |\hat{\varphi}(k) - \hat{\varphi}(0)| \leq \frac{\varepsilon}{4n} \quad \text{and} \quad \int_{|k| \leq \eta} \frac{(2\pi)^{-d} \hat{\varphi}(0) dk}{e^{\beta k^2} - 1} \leq \frac{\varepsilon}{4}.$$

The first condition on η yields

$$\left| \frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| \leq \eta}} \frac{\hat{\varphi}(k) - \hat{\varphi}(0)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} \right| \leq \frac{\varepsilon}{4},$$

then, the second condition on η implies

$$\limsup_{L \rightarrow \infty} \left| \frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| \leq \eta}} \frac{\hat{\varphi}(0)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} - (n - n_c) \hat{\varphi}(0) \right| \leq \frac{\varepsilon}{4}.$$

Hence

$$\limsup_{L \rightarrow \infty} \left| \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{\hat{\varphi}(k)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} - (n - n_c) \hat{\varphi}(k) - \int_{\mathbb{R}^d} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta k^2} - 1} \right| \leq \varepsilon,$$

and as this holds for any $\varepsilon > 0$, we get the result. \square

APPENDIX A. DEFINITION OF QUASIFREE STATES

For brevity, we write $\psi_j^\sharp := \psi^\sharp(x_j)$. We recall that the truncated expectations are defined via

$$\omega(\psi_1^\sharp \cdots \psi_n^\sharp) = \sum_{P_n} \prod_{J \in P_n} \omega^T(\prod_{j \in J} \psi_j^\sharp), \quad (91)$$

where P_n are partitions of the ordered set $\{1, \dots, n\}$ into ordered subsets.

We have $\mu(\psi) = \omega(\psi)$ and

$$\omega^T(\psi_1^\sharp \psi_2^\sharp) = \omega(\psi_1^\sharp \psi_2^\sharp) - \omega(\psi_1^\sharp) \omega(\psi_2^\sharp). \quad (92)$$

For quasifree states, the correlation functions $\omega(\psi_1^\sharp \cdots \psi_n^\sharp)$, with $n > 2$ can be expressed through $\omega(\psi^\sharp(x))$ and $\omega(\psi^\sharp(x) \psi^\sharp(y))$ according to the Wick formula. For example,

$$\omega(\psi_1^\sharp \psi_2^\sharp \psi_3^\sharp) = \omega(\psi_1^\sharp) \omega(\psi_2^\sharp \psi_3^\sharp) + \omega(\psi_2^\sharp) \omega(\psi_1^\sharp \psi_3^\sharp) + \omega(\psi_3^\sharp) \omega(\psi_1^\sharp \psi_2^\sharp) - 2 \prod_{i=1}^3 \omega(\psi_i^\sharp) \quad (93)$$

and

$$\omega(\psi_1^\# \psi_2^\# \psi_3^\# \psi_4^\#) = \omega(\psi_1^\# \psi_2^\#) \omega(\psi_3^\# \psi_4^\#) + \omega(\psi_1^\# \psi_3^\#) \omega(\psi_2^\# \psi_4^\#) + \omega(\psi_1^\# \psi_4^\#) \omega(\psi_2^\# \psi_3^\#) - 2 \prod_{i=1}^4 \omega(\psi_i^\#) \quad (94)$$

(remember that ψ 's stand on the right of ψ^* 's.) Note that

$$\omega(\psi^*(x)) = \overline{\omega(\psi(x))}, \quad \omega(\psi_1^* \psi_2^*) = \overline{\omega(\psi_2 \psi_1)}$$

and

$$\omega(\psi_1 \psi_2^*) = \omega(\psi_2^* \psi_1) + \delta(x - y).$$

Thus a quasifree state ω is completely determined by the functions $\omega(\psi(x))$, $\mu(\psi^*(x)\psi(y))$ and $\mu(\psi(x)\psi(y))$.

Remark A.1. *It is instructive to rewrite correlation functions for a quasifree state ω in terms of the fluctuation fields $\chi(x)$ which are defined as follows*

$$\psi = \phi + \chi, \quad \text{where } \phi(x) = \omega(\psi(x)), \quad (95)$$

the average field. Then ω is a quasifree state iff $\omega(\chi_1^\# \cdots \chi_{2n-1}^\#) = 0$ and

$$\omega(\chi_1^\# \cdots \chi_{2n}^\#) = \sum_{\pi \in S_n} \prod_{i=1}^{2n-1} \omega(\chi_{\pi(i)}^\# \chi_{\pi(i+1)}^\#),$$

where the sum is taken over all the permutations π of the set of indices $\{1, \dots, 2n\}$ satisfying $\pi(1) < \dots < \pi(2n)$.

APPENDIX B. DERIVATION OF THE BOSONIC HFB EQUATIONS

In this section, we prove Theorem 2.2. The derivations below are done in a somewhat informal way commonly used in dealing with operators on Fock spaces (see e.g. [3, 9, 17]). For instance, the commutator $[A, H]$, for $A = \psi(x)$ and $A = \psi(x)\psi(y)$, contains the terms $\Delta_x \psi(x)$ and $\psi(x)\Delta_y \psi(y)$. The formal computation gives $\omega^q(\Delta_x \psi(x)) = \Delta_x \omega^q(\psi(x))$ and $\omega^q(\psi(x)\Delta_y \psi(y)) = \Delta_y \omega^q(\psi(x)\psi(y))$, which are well-defined by our assumptions and are equal to $\Delta_x \phi(x)$ and $\Delta_y \sigma(x, y)$, respectively.

To do this more carefully, one uses, instead of operator functions $\psi^\#(x)$, the operator functionals $\psi^\#(f)$, for some nice f . E.g., instead $[\psi(x), H]$, we consider the commutator $[\psi(f), H]$, for any nice f , and concentrate on the term $\psi(\Delta f)$ it contains. Clearly, ω^q is well defined on $\psi(\Delta f)$ and can be written as $\omega^q(\psi(\Delta f)) = \int \overline{\Delta f}(x) \omega^q(\psi(x)) = \int \Delta \overline{f}(x) \phi(x) = \int \overline{f}(x) \Delta \phi(x)$. Thus we obtain the same result as above but in a weak form.

Proof of Theorem 2.2. We first observe that the three following condition are equivalent:

- (1) A quasifree state ω_t^q satisfies

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]), \quad (96)$$

for any operator \mathbb{A} of order ≤ 2 in the fields.

(2) A quasifree state ω_t^q satisfies

$$i\partial_t \omega_t^q(\psi(x)) = \omega_t^q([\psi(x), \mathbb{H}]) , \quad (97)$$

$$i\partial_t \omega_t^q(\psi^*(y)\psi(x)) = \omega_t^q([\psi^*(y)\psi(x), \mathbb{H}]) , \quad (98)$$

$$i\partial_t \omega_t^q(\psi(x)\psi(y)) = \omega_t^q([\psi(x)\psi(y), \mathbb{H}]) . \quad (99)$$

(3) A quasifree state ω_t^q with truncated expectations ϕ_t , γ_t and σ_t satisfies

$$i\partial_t \phi_t(x) = \omega_t^q([\psi(x), \mathbb{H}]) , \quad (100)$$

$$i\partial_t \gamma_t(x; y) = \omega_t^q([\psi^*(y)\psi(x), \mathbb{H}]) - i\partial_t(\phi_t(x)\overline{\phi_t(y)}) , \quad (101)$$

$$i\partial_t \sigma_t(x, y) = \omega_t^q([\psi(x)\psi(y), \mathbb{H}]) - i\partial_t(\phi_t(x)\phi_t(y)) . \quad (102)$$

We now suppose ω_t^q satisfies (100) - (102). Using the definition of the Hamiltonian, we obtain

$$\begin{aligned} i\partial_t \phi_t(x) &= \omega_t^q\left([\psi(x), \int \psi^*(y)h(y; y')\psi(y') dy dy']\right) \\ &\quad + \frac{1}{2}[\psi(x), \int v(y - y')\psi^*(y)\psi^*(y')\psi(y')\psi(y) dy dy'] \end{aligned} \quad (103)$$

$$= \omega_t^q\left(\int h(x; y')\psi(y') dy' + \int v(x - y)\psi^*(y)\psi(y)\psi(x) dy\right) , \quad (104)$$

where we used the CCR (3) to get

$$\begin{aligned} &[\psi(x), \psi^*(y)\psi^*(y')\psi(y')\psi(y)] \\ &= \delta(x - y)\psi^*(y')\psi(y')\psi(y) + \delta(x - y')\psi^*(y)\psi(y)\psi(y') . \end{aligned} \quad (105)$$

As ω_t^q is a quasifree state (see Appendix A)

$$\begin{aligned} \omega_t^q(\psi^*(y)\psi(y)\psi(x)) \\ = |\phi_t(y)|^2 \phi_t(x) + \sigma(y; x)\bar{\phi}_t(y) + \phi_t(x)\gamma(y; y) + \phi_t(y)\gamma(x; y) . \end{aligned} \quad (106)$$

We thus deduce that

$$\begin{aligned} i\partial_t \phi_t(x) &= \int h(x; y')\phi_t(y') dy' \\ &\quad + \int v(y - x)\phi_t(x)\gamma_t(y; y) dy + \int v(y - x)\phi_t(y)\gamma_t(x; y) dy \\ &\quad + \int v(x - y)\sigma_t(y, x)\bar{\phi}_t(y) dy + \int v(y - x)\phi_t(y)\phi_t(x)\bar{\phi}_t(y) dy \\ &= ((h + b[\gamma_t])\phi_t)(x) + k(\sigma_t^{\phi_t})\bar{\phi}_t(x) \end{aligned}$$

which is the dynamical equation (26) for ϕ_t .

For γ_t and σ_t , instead of ω_t^q we use

$$\omega_{C,t}^q(\mathbb{A}) := \omega_t^q(W_{\phi_t} \mathbb{A} W_{\phi_t}^*) , \quad (107)$$

where, recall, $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$, the Weyl operators, which satisfy

$$W_\phi^* \psi(x) W_\phi = \psi(x) + \phi(x) . \quad (108)$$

Note that the state $\omega_{C,t}^q$ is quasifree because ω_t^q is quasifree. By construction $\omega_{C,t}^q(\psi(x)) = 0$ and thus using (5) and the quasifreeness of $\omega_{C,t}^q$ one sees that

$\omega_{C,t}^q$ vanishes on monomials of odd order in the fields. This provides substantial simplifications in the computations below.

In particular the equations of the dynamics for γ_t and σ_t can be rewritten

$$i\partial_t \gamma_t(x; y) = \omega_{C,t}^q([\psi^*(y)\psi(x), W_{\phi_t}^* \mathbb{H}W_{\phi_t}]) , \quad (109)$$

$$i\partial_t \sigma_t(x_1, y) = \omega_{C,t}^q([\psi(x_1)\psi(y), W_{\phi_t}^* \mathbb{H}W_{\phi_t}]) . \quad (110)$$

We compute $W_{\phi_t}^* \mathbb{H}W_{\phi_t}$ modulo terms of odd degree and of degree 0 in the creation and annihilation operators:

$$\begin{aligned} W_{\phi_t}^* \mathbb{H}W_{\phi_t} &\equiv \int \psi^*(z)(h + b_v[|\phi\rangle\langle\phi|])(z; z')\psi(z') dz dz' \\ &\quad + \frac{1}{2} \int v(z - z')\phi_t(z)\phi_t(z')\psi^*(z)\psi^*(z') dz dz' + adj. \\ &\quad + \frac{1}{2} \int v(z - z')\psi^*(z)\psi^*(z')\psi(z')\psi(z) dz dz' . \end{aligned} \quad (111)$$

Because $\omega_{C,t}^q$ vanishes on monomials of odd order in the fields and using the commutator, the knowledge of $W_{\phi_t}^* \mathbb{H}W_{\phi_t}$ modulo terms of odd degree and of degree 0 in the creation and annihilation operators is sufficient to compute the time derivative (109) of γ_t . Thus using the CCR we get

$$\begin{aligned} i\partial_t \gamma_t(x; y) &= \int \omega_{C,t}^q \left((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z)\psi^*(y)\psi(z) \right. \\ &\quad - (h + b_v[|\phi_t\rangle\langle\phi_t|])(z; y)\psi^*(z)\psi(x) \\ &\quad + v(z - x)\phi_t(z)\phi_t(x)\psi^*(y)\psi^*(z) - v(z - y)\overline{\phi_t(z)\phi_t(y)}\psi(z)\psi(x) \\ &\quad \left. + v(z - x)\psi^*(y)\psi^*(z)\psi(x)\psi(z) - v(z - y)\psi^*(z)\psi^*(y)\psi(z)\psi(x) \right) dz . \end{aligned} \quad (112)$$

From the quasifreeness of $\omega_{C,t}^q$ follows

$$\begin{aligned} i\partial_t \gamma_t(x; y) &= [h + b_v[|\phi_t\rangle\langle\phi_t| + \gamma_t], \gamma_t](x; y) \\ &\quad + \int (v(z - x)\phi_t(z)\phi_t(x)\overline{\sigma_t(y, z)} - v(z - y)\overline{\phi_t(z)\phi_t(y)}\sigma_t(z, x) \\ &\quad + v(z - x)\sigma_t(x, z)\overline{\sigma_t(y, z)} - v(z - y)\sigma_t(x, z)\overline{\sigma_t(y, z)}) dz . \end{aligned} \quad (113)$$

which is the dynamical equation (27) for γ_t .

Using the same arguments as for γ_t , we get

$$\begin{aligned} i\partial_t \sigma_t(x; y) &= \omega_{C,t}^q \left(v(x - y)\phi_t(x)\phi_t(y) + v(x - y)\psi(x)\psi(y) \right. \\ &\quad + \int ((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z)\psi(y)\psi(z) + (h + b_v[|\phi_t\rangle\langle\phi_t|])(y; z)\psi(x))\psi(z) \\ &\quad + v(x - z)\psi^*(z)\psi(y)\phi_t(x)\phi_t(z) + v(y - z)\psi^*(z)\psi(x)\phi_t(y)\phi_t(z) \\ &\quad \left. + v(x - z)\psi^*(z)\psi(y)\psi(x)\psi(z) + v(y - z)\psi^*(z)\psi(x)\psi(y)\psi(z) \right) dz . \end{aligned} \quad (114)$$

From the quasifreeness of $\omega_{C,t}^q$ follows

$$\begin{aligned}
i\partial_t \sigma_t(x; y) &= v(x-y)\phi_t(x)\phi_t(y) + v(x-y)\sigma_t(x, y) \\
&+ \int \left((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z)\sigma_t(y, z) + (h + b_v[|\phi_t\rangle\langle\phi_t|])(y; z)\sigma_t(x, z) \right. \\
&+ v(x-z)\gamma_t(y; z)\phi_t(x)\phi_t(z) + v(y-z)\gamma_t(x; z)\phi_t(y)\phi_t(z) \\
&+ v(x-z)(\gamma_t(x; z)\sigma_t(z, y) + \gamma_t(y; z)\sigma_t(z, x) + \gamma_t(z; z)\sigma_t(x, y)) \\
&\left. + v(y-z)(\gamma_t(x; z)\sigma_t(z, y) + \gamma_t(y; z)\sigma_t(z, x) + \gamma_t(z; z)\sigma_t(x, y)) \right) dz, \quad (115)
\end{aligned}$$

which is the dynamical equation (28) for σ_t . \square

APPENDIX C. EQUIVALENCE OF THE HFB EQUATIONS WITH THE EVOLUTION GENERATED BY $\mathbb{H}_{hfb}(\omega_t^q)$

In this section, we prove Theorem 2.4.

Let a quasifree state ω_t^q satisfy (32) and let ϕ_t, γ_t and σ_t denote its truncated expectations. Below, we use the abbreviations $h(t) \equiv h(\gamma_t^{\phi_t})$ and $k(t) \equiv k(\sigma_t^{\phi_t})$, where, recall, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + |\phi\rangle\langle\phi|$, and $h(\gamma)$ and $k(\sigma)$ are defined in (29) and (30). To find the equation for ϕ_t , we compute

$$\begin{aligned}
i\partial_t \phi_t(x) &= \omega_t^q([\psi(x), \mathbb{H}_{hfb}(\omega_t^q)]) \\
&= \tilde{\omega}_t^q \left(\int h(t)(x; z)\psi(z)dz - b[|\phi_t\rangle\langle\phi_t|]\phi_t(x) + \int \psi^*(z)k(t)(x, z)dz \right) \\
&= h(t)\phi_t(x) - b[|\phi_t\rangle\langle\phi_t|]\phi_t(x) + k(t)\overline{\phi_t}(x).
\end{aligned}$$

Hence ϕ_t satisfies (26).

For γ_t and σ_t we remark that, modulo terms of order one and constants $W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t}$ and $\mathbb{H}_{hfb}(\omega_t^q)$ coincide, hence

$$\begin{aligned}
W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t} &\equiv \int h(t)(z; z')\psi^*(z)\psi(z')dzdz' \\
&+ \frac{1}{2} \int \psi^*(z_1)\psi^*(z_2)k(t)(z_1, z_2)dz_1dz_2 + adj. \quad (116)
\end{aligned}$$

Recall the definition (107) of $\omega_{C,t}^q(\mathbb{A})$. As in the proof of Theorem 2.2 the terms coming from the derivative of W_{ϕ_t} simplify:

$$i\partial_t \gamma_t(x; y) = \omega_{C,t}^q([\psi^*(y)\psi(x), W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t}]).$$

It is sufficient to consider $W_{\phi_t}^* \tilde{\mathbb{H}}(\phi_t, \gamma_t, \sigma_t) W_{\phi_t}$ modulo monomials of odd order in the fields:

$$\begin{aligned} i\partial_t \gamma_t(x; y) &= \omega_{C,t}^q \left(\int h(t)(x; z) \psi^*(x) \psi(z) dz - \int h(t)(z; y) \psi^*(z) \psi(y) dz \right. \\ &\quad \left. + \int \psi^*(z) \psi^*(y) k(t)(z, x) dz - \int \overline{k(t)(z, y)} \psi(z) \psi(x) dz \right) \\ &= \int h(t)(x; z) \gamma_t(z; x) dz - \int \gamma_t(x; z) h_v(t)(z; y) dz \\ &\quad + \int \overline{\sigma_t(y, z)} k(t)(z, x) dz - \int \overline{k(t)(z, y)} \sigma_t(x, z) dz. \end{aligned}$$

Similarly

$$i\partial_t \sigma_t(x; y) = \omega_{C,t}^q ([\psi(x) \psi(y), W_{\phi_t}^* \mathbb{H}_{hb}(\omega_t^q) W_{\phi_t}]) \quad (117)$$

and

$$\begin{aligned} i\partial_t \gamma_t(x; y) &= \int h(t)(x; z) \sigma_t(x, z) dz + \int h(t)(y; z) \sigma_t(y, z) dz \\ &\quad + \int \gamma_t(y, z) k(t)(z, x) dz + \int \gamma_t(x, z) k(t)(z, y) dz + k(t)(x, y) \end{aligned} \quad (118)$$

Thus γ_t and σ_t satisfy (27) and (28).

We have shown that, if a quasifree state ω_t^q satisfies (32), then its truncated expectations, ϕ_t, γ_t and σ_t , satisfy (26), (27) and (28). Proceeding in the opposite direction, one shows that, if truncated expectations, ϕ_t, γ_t and σ_t , satisfy (26), (27) and (28), then the corresponding quasifree state ω_t^q satisfies (32). \square

APPENDIX D. SELF-ADJOINTNESS OF THE HAMILTONIAN \mathbb{H}

The assumption $v^2 \leq C(1 - \Delta)$ ensures that the original Hamiltonian \mathbb{H} in (1) is self-adjoint, although not necessarily semi-bounded. In fact the same arguments as those used to prove (74) allow to deduce

$$\mathbb{V} \leq C(\mathbb{T} + \mathbb{N}^3) \quad (119)$$

with \mathbb{V} defined in (74), \mathbb{T} defined in (70), from

$$|v| \leq \sqrt{C(1 - \Delta)} \leq \varepsilon(1 - \Delta) + C_1 \varepsilon^{-1} \leq -\varepsilon \Delta + C_2 \varepsilon^{-1}. \quad (120)$$

for some $C_j > 0$. One can then use the KLMN theorem and the Nelson theorem (see [34, 30]) to prove the self-adjointness of \mathbb{H} . (Details can be adapted from, e.g., [1, Section 3].)

APPENDIX E. OPERATORS b AND k

Lemma E.1. *Assume that the pair interaction potential v is symmetric, $v(x) = v(-x)$, and such that $v^2 \leq CM^2$ for some $C > 0$.*

Then, the operators b and k defined in (29) and (30) possess the following properties:

- (1) b is linear and continuous from \mathcal{H}^1 to $\mathcal{B}(H^1) \simeq MB(L^2)M^{-1}$.
- (2) k is linear and continuous from H_s^1 to $M\mathcal{L}^2(L^2)M^{-1}$.

Proof. The linearity is clear. For the detailed proof of statement (1), we refer to [7]. For the reader's convenience, we recall here the main arguments.

For statement (1), we first consider the direct term, i.e., the first term in the definition of b . It is sufficient to prove that $v * n$ (with $n(x) = \gamma(x; x)$) and $\nabla v * n$ are functions uniformly bounded by $\|\gamma\|_{\mathcal{H}^1}$. As those two bounds are very similar, we focus on the more difficult one, $\nabla v * n$. Note that γ can be decomposed as $\gamma = \sum_{j=1}^{\infty} \lambda_j |\varphi_j\rangle\langle\varphi_j|$ with $\lambda_j \geq 0$. Using this decomposition, combined with the Cauchy-Schwarz inequality, we find

$$\begin{aligned} \left\| \nabla_x \int_{\mathbb{R}^d} v(x-y) \gamma(y; y) dy \right\|_{\infty} &\leq \sum_{j=1}^{\infty} \lambda_j \left\| \int_{\mathbb{R}^d} |v(x-y)| |\varphi_j(y)| \nabla \varphi_j(y) dy \right\|_{\infty} \\ &\leq \sum_{j=1}^{\infty} \lambda_j \left\| \left(\int_{\mathbb{R}^d} v(x-y)^2 |\varphi_j(y)|^2 dy \right)^{1/2} \nabla \varphi_j \right\|_{L^2(\mathbb{R}^d)} \left\| \nabla \varphi_j \right\|_{L^2(\mathbb{R}^d)} \left\| \nabla \varphi_j \right\|_{L^2(\mathbb{R}^d)} \\ &\leq \sum_{j=1}^{\infty} \lambda_j \sqrt{C} \|M \varphi_j\|_{L^2(\mathbb{R}^d)}^2 \leq \sqrt{C} \|\gamma\|_{\mathcal{H}^1} \end{aligned}$$

The estimates for the exchange term (the second term in the definition of B) are similar.

For Point (2). We observe that $v(x-y)^2 \leq C M_y^2$ on symmetric functions thanks to $v^2 \leq C M^2$, the translation invariance of M and the symmetry. Inverting¹ this relation yields $M_y^{-2} \leq C v(x-y)^2$. Then, using the relation $\|k[\sigma]\|_{M\mathcal{L}^2(L^2)M^{-1}} = \|Mk[\sigma]M^{-1}\|_{L^2(\mathbb{R}^{2d})}^2$, we prove the continuity of k :

$$\begin{aligned} \|k[\sigma]\|_{M\mathcal{L}^2(L^2)M^{-1}} &= \langle v(x-y)\sigma(x, y), M_y^{-2}v(x-y)\sigma(x, y) \rangle \\ &\quad + \langle \nabla_x(v(x-y)\sigma(x, y)), M_y^{-2}\nabla_x(v(x-y)\sigma(x, y)) \rangle, \quad (121) \end{aligned}$$

where the first term is smaller than $C\|\sigma\|_{L^2(\mathbb{R}^{2d})}^2$ because of $M_y^{-2} \leq C v(x-y)^{-2}$. Computing the derivatives in the scalar product on the right-hand side of the inequality allows to estimate it by the quantity below:

$$\begin{aligned} &2\langle (\nabla v)(x-y)\sigma(x, y), M_y^{-2}(\nabla v)(x-y)\sigma(x, y) \rangle \\ &\quad + 2\langle v(x-y)(\nabla_x \sigma)(x, y), M_y^{-2}v(x-y)(\nabla_x \sigma)(x, y) \rangle \\ &\leq 2\langle \sigma(x, y), v^2(x-y)\sigma(x, y) \rangle + 2\langle (\nabla_x \sigma)(x, y), (\nabla_x \sigma)(x, y) \rangle. \end{aligned}$$

This yields the result as the last line is controlled by $4C\|\sigma\|_{H_s^1}^2$. \square

¹See [4] Proposition V.1.6 where the result is stated for matrices, but the proof can be extended to operators.

REFERENCES

- [1] Z. Ammari and S. Breteaux. Propagation of chaos for many-boson systems in one dimension with a point pair-interaction. *Asymptot. Anal.*, 76(3-4):123–170, 2012. doi: 10.3233/ASY-2011-1064.
- [2] V. Bach and J.-B. Bru. Diagonalizing quadratic bosonic operators by non-autonomous flow equation. *Mem. Amer. Math. Soc.*, 240(1138), 2015. doi: 10.1090/memo/1138.
- [3] F. A. Berezin. *The method of second quantization*. Translated from the Russian by Nobumichi Mugibayashi and Alan Jeffrey. Pure and Applied Physics, Vol. 24. Academic Press, 1966.
- [4] R. Bhatia. *Matrix analysis*, volume 169 of *Graduate Texts in Mathematics*. Springer-Verlag, 1997. doi: 10.1007/978-1-4612-0653-8.
- [5] F. Bloch. Nuclear Induction. *Phys. Rev.*, 70:460–474, 1946. doi: 10.1103/PhysRev.70.460.
- [6] A. Bove, G. Da Prato, and G. Fano. An existence proof for the Hartree-Fock time-dependent problem with bounded two-body interaction. *Comm. Math. Phys.*, 37:183–191, 1974. <http://projecteuclid.org/euclid.cmp/1103859879>.
- [7] A. Bove, G. Da Prato, and G. Fano. On the Hartree-Fock time-dependent problem. *Comm. Math. Phys.*, 49(1):25–33, 1976. <http://projecteuclid.org/euclid.cmp/1103899939>.
- [8] O. Bratteli and D. W. Robinson. *Operator algebras and quantum statistical mechanics. Vol. 1*. Springer-Verlag, 1979. doi: 10.1007/978-3-662-02520-8.
- [9] O. Bratteli and D. W. Robinson. *Operator algebras and quantum-statistical mechanics. II*. Springer-Verlag, 1981. doi: 10.1007/978-3-662-03444-6.
- [10] T. Cazenave and A. Haraux. *An introduction to semilinear evolution equations*, volume 13 of *Oxford Lecture Series in Mathematics and its Applications*. The Clarendon Press, Oxford University Press, 1998.
- [11] J. M. Chadam. The time-dependent Hartree-Fock equations with Coulomb two-body interaction. *Comm. Math. Phys.*, 46(2):99–104, 1976. <http://projecteuclid.org/euclid.cmp/1103899583>.
- [12] J. M. Chadam and R. T. Glassey. Global existence of solutions to the Cauchy problem for time-dependent Hartree equations. *J. Math. Phys.*, 16:1122–1130, 1975. doi: 10.1063/1.522642.
- [13] R. H. Critchley and A. Solomon. A Variational Approach to Superfluidity. *J. Stat. Phys.*, 14:381–393, 1976. doi: 10.1007/BF01030201.
- [14] R. J. Dodd, M. Edwards, C. W. Clark, and K. Burnett. Collective excitations of Bose-Einstein-condensed gases at finite temperatures. *Phys. Rev. A*, 57:R32–R35, 1998. doi: 10.1103/PhysRevA.57.R32.
- [15] A. Griffin. Conserving and gapless approximations for an inhomogeneous Bose gas at finite temperatures. *Phys. Rev. B*, 53:9341–9347, 1996. doi: 10.1103/PhysRevB.53.9341.
- [16] M. Grillakis and M. Machedon. Pair excitations and the mean field approximation of interacting Bosons, II. *ArXiv e-prints*, September 2015. <http://arxiv.org/abs/1509.05911>.
- [17] S. J. Gustafson and I. M. Sigal. *Mathematical concepts of quantum mechanics*. Universitext. Springer, second edition, 2011. doi: 10.1007/978-3-642-21866-8.

- [18] T. Kato. Linear evolution equations of “hyperbolic” type. *J. Fac. Sci. Univ. Tokyo Sect. I*, 17:241–258, 1970.
- [19] L. Landau. Das Dämpfungsproblem in der Wellenmechanik. *Zeitschrift für Physik*, 45(5):430–441, 1927. doi: 10.1007/BF01343064.
- [20] M. Lewin. Mean-field limit of Bose systems: rigorous results. *ArXiv e-prints*, October 2015. <http://arxiv.org/abs/1510.04407>.
- [21] M. Lewin, P. T. Nam, and N. Rougerie. The mean-field approximation and the non-linear Schrödinger functional for trapped Bose gases. *Trans. Amer. Math. Soc.*, In press. doi: 10.1090/tran/6537.
- [22] M. Lewin, P. T. Nam, and N. Rougerie. A note on 2D focusing many-boson systems. *ArXiv e-prints*, September 2015. <http://arxiv.org/abs/1509.09045>.
- [23] M. Lewin, P. T. Nam, and B. Schlein. Fluctuations around Hartree states in the mean-field regime. *Am. J. Math.*, 137(6):1613–1650, 2015. doi: 10.1353/ajm.2015.0040.
- [24] R. McOwen. *Partial Differential Equations. Methods and Applications*. Prentice-Hall, 2nd edition, 2003.
- [25] M. Merkli, M. Mück, and I. M. Sigal. Theory of Non-Equilibrium Stationary States as a Theory of Resonances. *Annales Henri Poincaré*, 8(8):1539–1593, 2007. doi: 10.1007/s00023-007-0346-4.
- [26] P. T. Nam and M. Napiórkowski. Bogoliubov correction to the mean-field dynamics of interacting bosons. *ArXiv e-prints*, September 2015. <http://arxiv.org/abs/1509.04631>.
- [27] P. T. Nam, M. Napiórkowski, and J. P. Solovej. Diagonalization of bosonic quadratic Hamiltonians by Bogoliubov transformations. *ArXiv e-prints*, August 2015. <http://arxiv.org/abs/1508.07321>.
- [28] M. Napiórkowski, R. Reuvers, and J. P. Solovej. The Bogoliubov free energy functional I. Existence of minimizers and phase diagram. *ArXiv e-prints*, November 2015. <http://arxiv.org/abs/1511.05935>.
- [29] M. Napiórkowski, R. Reuvers, and J. P. Solovej. The Bogoliubov free energy functional II. The dilute limit. *ArXiv e-prints*, November 2015. <http://arxiv.org/abs/1511.05953>.
- [30] E. Nelson. Time-ordered operator products of sharp-time quadratic forms. *J. Functional Analysis*, 11:211–219, 1972. doi: 10.1016/0022-1236(72)90091-2.
- [31] J. von Neumann. Wahrscheinlichkeitstheoretischer Aufbau der Quantenmechanik. *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, 1927:245–272, 1927. <http://eudml.org/doc/59230>.
- [32] A. S. Parkins and D. F. Walls. The physics of trapped dilute-gas Bose–Einstein condensates. *Phys. Rep.*, 303(1):1–80, 1998. doi: 10.1016/S0370-1573(98)00014-3.
- [33] W. Pauli. *Probleme der modernen Physik*. S. Hirzel, Leipzig, 1928.
- [34] M. Reed and B. Simon. *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*. Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975.
- [35] I. Segal. Non-Linear Semi-Groups. *Ann. Math.*, 78(2):pp. 339–364, 1963. doi: 10.2307/1970347.
- [36] D. Shale. Linear symmetries of free boson fields. *Trans. Amer. Math. Soc.*, 103:149–167, 1962. doi: 10.1090/S0002-9947-1962-0137504-6.

- [37] D. ter Haar. *Men of Physics: L.D. Landau*, volume 2: Thermodynamics, Plasma Physics and Quantum Mechanics. Pergamon Press, 1969.
- [38] S. Zagatti. The Cauchy problem for Hartree-Fock time-dependent equations. *Ann. Inst. H. Poincaré Phys. Théor.*, 56(4):357–374, 1992.
http://www.numdam.org/item?id=AIHPA_1992__56_4_357_0.

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